UNIVERSITY OF SOUTHAMPTON

Faculty of Social and Human Sciences

School of Mathematics

Screening experiments using supersaturated designs with application to industry

by

Christopher James Marley

Thesis for the degree of Doctor of Philosophy

November 2010

UNIVERSITY OF SOUTHAMPTON

ABSTRACT

FACULTY OF SOCIAL AND HUMAN SCIENCES

SCHOOL OF MATHEMATICS

Doctor of Philosophy

SCREENING EXPERIMENTS USING SUPERSATURATED DESIGNS WITH APPLICATION TO INDUSTRY

by Christopher James Marley

This thesis describes the statistical methodology behind a variety of industrial screening experiments. The primary focus of the thesis is on supersaturated designs that have more parameters to be investigated than runs available. Such designs are particularly useful when experiments are expensive to perform. In addition, the statistical issues behind a real-life screening experiment are investigated, where there is a functional response and the factor levels cannot be set directly.

A study to compare several existing design and analysis methods for two-level supersaturated designs was carried out. A variety of different scenarios in terms of numbers of runs, numbers of factors and numbers of active factors were investigated via simulated experiments. The Gauss-Dantzig selector was identified as an effective analysis method, whilst little difference was found in the practical performance of designs from the different criteria. As a result of the study, several guidelines are provided, to indicate when supersaturated designs are most likely to be effective as a screening tool.

A new criterion for designing supersaturated experiments under measures of multicollinearity is presented. The criterion is particularly applicable to experiments where factor levels cannot be set independently, although its application to two-level designs is also demonstrated. An optimal allocation of factors to columns of an existing design is also considered.

Supersaturated experiments are discussed in the context of robust product design, where the interactions between control factors and noise factors are explored. A new criterion specifically applicable to supersaturated robust product design experiments is described. The fact that the experimenter is interested in some parameters more than others is exploited and the cost savings from using a supersaturated experiment are illustrated. It is demonstrated that substantial gains in power to detect active effects can be achieved when using this new criterion.

Finally, the design and analysis of a practical screening experiment is discussed. Complicating features of the experiment include the multivariate nature of the response and the fact that factor levels cannot be set directly. A two-stage linear mixed effect model is applied, with principal components analysis used for the first-stage models. A novel method for finding follow-up runs to the screening experiment is described and implemented.

Contents

List of Figures

List of Tables

List of Accompanying Material

- CD containing a catalogue of effect-focussed $E(s^2)$ designs described in Chapter 4. Control factors are denoted by capital letters and noise factors by lower case letters.

Declaration of authorship

I, **Christopher Marley**, declare that the thesis entitled **Screening experiments using supersaturated designs with application to industry** and the work presented in the thesis are both my own, and have been generated by me as the result of my own original research. I confirm that:

- this work was done wholly or mainly while in candidature for a research degree at this University;
- where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated;
- where I have consulted the published work of others, this is always clearly attributed;
- where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work;
- I have acknowledged all main sources of help;
- where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself;
- parts of this work have been published as:

  Marley, C.J. and Woods, D.C. (2010). A comparison of design and model selection methods for supersaturated experiments. Computational Statistics and Data Analysis, 54, 3158-3167.

Signed:

Date:

Acknowledgments

I would like to thank my supervisor, Dr David Woods, and my advisor Professor Susan Lewis, for their sustained guidance, enthusiasm and support throughout the compilation of this thesis. I would also like to thank Professor Dennis Lin for his encouragement and advice relating to Chapter 4 of this thesis, and also for his kindness during my visit to Penn State. I am grateful for the funding from EPSRC and acknowledge the generous support of the Lubrizol Corporation throughout my PhD, in particular the assistance of Dr Andrew Rose, Dr Michael Gahagan, John Durham, Dr Oliver Smith and Dr Robert Wilkinson with the case study in Chapter 5. Finally, thanks go to Dr John Fenlon for introducing me to the area of Design of Experiments.

Chapter 1

Introduction

There are often many different variables, or factors which could potentially affect the performance of a product or process. However, in reality, we expect only a small number of these factors to have a substantive impact on the response(s) of interest. This concept is known as *effect sparsity* (Box and Meyer, 1986). Screening is the process of using designed experiments and statistical analysis to establish which of these many factors have a substantive impact on the response(s) of interest.

Following the screening procedure, follow-up experiments involving fewer variables are performed to enable the fitting of a more precise model and to validate the findings at the screening stage (see for instance Meyer et al., 1996). This is more cost effective than performing a much larger number of runs at the first stage, when many more factors are under consideration.

The model used for screening experiments is typically of the form

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}\,,$$

where $\mathbf{Y}$ is the response vector, $\mathbf{X}$ is a model matrix, $\boldsymbol{\beta}$ is a vector of unknown coefficients and $\boldsymbol{\varepsilon}$ is a vector of independent normally distributed random errors with mean 0 and variance σ^2. The model matrix $\mathbf{X}$ will typically only incorporate an intercept and main effects, although sometimes two-factor interactions are investigated. As such, experiments typically take place with the factors having two levels, one high and one low, denoted by 1 and -1.

With a widening range of processes now under investigation in industry, and also an

increasing number of factors being explored as manufacturers look to improve the quality of their products, the importance of effective screening strategies is greater than ever.

Traditional methods of screening are full factorial and regular fractional factorial experiments (see for instance Wu and Hamada, 2000, ch. 3-4). Full factorial experiments are only utilised when the number of factors is small, since the number of runs rapidly becomes large as the number of factors increases. When there are a large number of factors, fractional factorial designs can result in very small and efficient experiments but still with more runs than factors *and* complete aliasing between effects potentially of interest.

Another method of screening is the use of non-regular fractions, where partial aliasing between some effects is present. Plackett-Burman designs (Plackett and Burman, 1946) are non-regular designs which can investigate up to m factors in $m + 1$ runs when the number of runs is a multiple of 4. They have all main effects orthogonal to each other, but partial aliasing between two-factor interactions occurs when the number of runs is not a power of 2 (when the design corresponds to a regular fraction).

Some experimenters use a group screening strategy, whereby the factors under investigation are partitioned into groups (Watson, 1961; Lewis and Dean, 2001). In each experimental run, all factors within a group are set to the same level. Thus, factors within the same group are completely confounded with each other at the screening stage, with corresponding impact on confounding between interactions. This approach is most effective when the directions of the possible effects are known, with only factors with the same directional effects being grouped together. For more recent developments, including multi-stage group screening and group screening involving interactions, see Morris (2006).

In this thesis we focus on the design and analysis of supersaturated experiments (Booth and Cox, 1962; Lin, 1993; Wu, 1993). In certain experiments, particularly in the manufacturing industry, the cost of a single run can be very high. Hence there are very strict constraints on the number of runs that can be performed. However, subject experts may produce a list of many factors which they think could

potentially affect the response under investigation. In order to investigate all of these factors, the experimenter may wish to use a supersaturated design. This is traditionally defined as a design which has fewer runs than factors to be investigated, although a more general definition that there are more parameters of interest than runs available is sometimes adopted. As a consequence, there are several challenging issues involved in designing and analysing this type of experiment.

For a thorough review of screening strategies, see Dean and Lewis (2006).

When designing an experiment, our philosophy is that no effects of interest should be completely confounded, that is, our design should provide some information on all the parameters in the model. For supersaturated experiments we consider both

(i) how to design the experiment, including both design criteria and construction methods, and

(ii) how to analyse the resulting data.

In addition, we provide guidance on the situations from which you are most likely to see good performance from using a supersaturated experiment.

This thesis is structured as four independent contributing chapters, along with an introduction and discussion chapter. The four contributing chapters are self contained, with independent notation for each, and no cross-referencing between them.

Chapter 2 of this thesis compares different methods for the design and analysis of supersaturated experiments. A new analysis method is also proposed and compared to existing methods. Further to this, the performance of different sizes of supersaturated experiments under several scenarios, involving different numbers and sizes of active effects, is investigated, enabling recommendations to be made on when the practical implementation of supersaturated experiments is most likely to be successful.

Chapter 3 describes a new class of criteria for designing supersaturated experiments. This differs from most existing criteria in that it considers projections into subsets of more than two factors. The criteria are used to generate several new two-level supersaturated designs. Designs were also found for the case where factor levels

cannot be set independently, which has been little addressed in the literature. Such a situation can occur when experimenting with chemical compounds. The new set of criteria are particularly applicable to such an experiment, and examples are presented to illustrate this. We also apply the criteria to assigning factors to columns in existing supersaturated designs when some prior information is available.

Chapter 4 develops a new criterion for selecting supersaturated designs for robust product design, exploiting interactions between control factors, which can be set in the product specification, and noise factors, which cannot, but can be mimicked in an experiment. Designs are generated and catalogued for many combinations of control and noise factors. The benefits of these designs are illustrated by comparing their performance against other designs in simulation studies.

Chapter 5 describes the design and analysis of a real screening experiment at the specialty chemicals company Lubrizol. The experiment investigates the impact of oil formulation and process variables on the friction between surfaces. The equipment used is designed to mimic the friction and wear that may be experienced for instance in an engine or gearbox. The output from each run of the experiment is a curve and there are further statistical complications resulting from constraints on the design space. A new method for choosing appropriate follow-up runs to the screening experiment is described and implemented.

Chapter 2

A comparison of design and model selection methods for supersaturated experiments

Various design and model selection methods are available for supersaturated designs having more factors than runs but little research is available on their comparison and evaluation. Simulated experiments are used to evaluate the use of $E(s^2)$-optimal and Bayesian D-optimal designs and to compare four analysis strategies representing regression, shrinkage, orthogonal decomposition and a novel model averaging procedure. Suggestions are made for choosing the values of the tuning constants for each approach. Findings include that (i) the preferred analysis is via shrinkage; (ii) designs with similar numbers of runs and factors can be effective for a considerable number of active effects of only moderate size; and (iii) unbalanced designs can perform well. Some comments are made on the performance of the design and analysis methods when effect sparsity does not hold.

2.1 Introduction

A screening experiment investigates a large number of factors to find those with a substantial effect on the response of interest, that is, the active factors. If a large experiment is infeasible, then using a supersaturated design in which the number of factors exceeds the number of runs may be considered. This chapter investigates the performance of a variety of design and model selection methods for supersaturated experiments through simulation studies.

Supersaturated designs were first suggested by Box (1959) in the discussion of Satterthwaite (1959). Booth and Cox (1962) provided the first systematic construction method and made the columns of the design matrix as near orthogonal as possible through the $E(s^2)$ design selection criterion (see Section 2.2.1). Interest in design construction was revived by Lin (1993) and Wu (1993), who developed methods based on Hadamard matrices. Recent theoretical results for $E(s^2)$-optimal and highly efficient designs include those of Nguyen and Cheng (2008). The most flexible design construction methods are algorithmic: Lin (1995), Nguyen (1996) and Li and Wu (1997) constructed efficient designs for the $E(s^2)$ criterion. More recently, Ryan and Bulutoglu (2007) provided a wide selection of designs that achieved lower bounds on $E(s^2)$, and Jones et al. (2008) constructed designs using Bayesian D-optimality. For a review of supersaturated designs, see Gilmour (2006).

The challenges in the analysis of data from supersaturated designs arise from correlations between columns of the model matrix and the fact that the main effects of all the factors cannot be estimated simultaneously. Methods to overcome these problems include regression procedures, such as forward selection (Westfall et al., 1998), stepwise and all-subsets regression (Abraham et al., 1999), shrinkage methods, including the Smoothly Clipped Absolute Deviation procedure (Li and Lin, 2002) and the Dantzig selector (Phoa et al., 2009), and orthogonal decomposition methods (Georgiou, 2008). We compare the performances of one representative from each of these classes of techniques, together with a new model-averaging procedure. Strategies are suggested for choosing values of the tuning constants for each analysis method. It is widely accepted that the effectiveness of supersaturated designs in detecting active factors requires there being only a small number of such factors, a principle known as effect sparsity (Box and Meyer, 1986).

Previous simulation studies compared either a small number of analysis methods (Li and Lin, 2003; Phoa et al., 2009) or different designs (Allen and Bernshteyn, 2003), usually for a narrow range of settings. In our simulations, several settings are explored with different numbers and sizes of active effects, and a variety of design sizes. The results lead to guidance on when supersaturated designs are effective screening tools.

In Section 2.2 we describe the design criteria and model selection methods investigated in the simulation studies. Section 2.3 describes the studies and summarises the results. Finally, in Section 2.4, we discuss the most interesting findings and draw some conclusions about the effectiveness of the methods for different numbers and sizes of active effects.

2.2 Design criteria and model selection methods

We consider a linear main effects model for the response

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}\,, \tag{2.1}$$

where $\mathbf{Y}$ is the $n \times 1$ response vector, $\mathbf{X}$ is an $n \times (m+1)$ model matrix, $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_m)^{\mathrm{T}}$ and $\boldsymbol{\varepsilon}$ is a vector of independent normally distributed random errors with mean 0 and variance σ^2. We assume that each of the m factors has two levels, ± 1. The first column of $\mathbf{X}$ is $\mathbf{1}_n = [1, \ldots, 1]^{\mathrm{T}}$, with column i corresponding to the levels of the $(i-1)$th factor $(i = 2, \ldots, m+1)$.

2.2.1 Design construction criteria

$E(s^2)$-optimality

Booth and Cox (1962) proposed a criterion that selects a design by minimising the sum of the squared inner products between columns i and j of $\mathbf{X}$ $(i, j = 2, \ldots, m+1;\, i \neq j)$. We extend this definition to include the inner product of the first column with every other column of $\mathbf{X}$ to give

$$E(s^2) = \frac{2}{m(m+1)} \sum_{i<j} s_{ij}^2\,, \tag{2.2}$$

where s_{ij} is the ijth element of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ $(i, j = 1, \ldots, m+1)$. The two definitions are equivalent for balanced designs, that is, where each factor is set to +1 and -1 equally often. The balanced $E(s^2)$-optimal designs used in this chapter were found using the algorithm of Ryan and Bulutoglu (2007). These designs achieve the lower bound on

$E(s^2)$ for balanced designs given by these authors and, where more than one design satisfies the bound, a secondary criterion of minimising $\max_{i<j} s_{ij}^2$ is employed.

Bayesian D-optimality

Under a Bayesian paradigm with conjugate prior distributions for $\boldsymbol{\beta}$ and σ^2 (O'Hagan and Forster, 2004, ch. 11), the posterior variance-covariance matrix for $\boldsymbol{\beta}$ is proportional to $(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \mathbf{K}/\tau^2)^{-1}$. Here, $\tau^2\mathbf{K}^{-1}$ is proportional to the prior variance-covariance matrix for $\boldsymbol{\beta}$. Jones et al. (2008) suggested finding a supersaturated design that maximises

$$\phi_D = |\mathbf{X}^{\mathrm{T}}\mathbf{X} + \mathbf{K}/\tau^2|^{1/(m+1)} .$$

They regarded the intercept β_0 as a *primary* term with large prior variance, and $\beta_1, \ldots, \beta_m$ as *potential* terms with small prior variances, see DuMouchel and Jones (1994), and set

$$\mathbf{K} = \begin{pmatrix} 0 & \mathbf{0}_{1\times m} \\ \mathbf{0}_{m\times 1} & \mathbf{I}_{m\times m} \end{pmatrix} . \tag{2.3}$$

The prior information can be viewed as equivalent to having sufficient additional runs to allow estimation of all factor effects. This method can generate supersaturated designs for any design size and any number of factors.

Bayesian D-optimal designs may be generated using a coordinate-exchange algorithm (Meyer and Nachtsheim, 1995). The value of τ^2 reflects the quantity of prior information; $\tau^2 = 1$ was used to obtain the designs presented. An assessment (not shown) of designs found for $\tau^2 = 0.2$ and $\tau^2 = 5$ indicated insensitivity of design performance to τ^2; see also Jones et al. (2008).

2.2.2 Model selection methods

Four methods are examined: regression (forward selection), shrinkage (Gauss-Dantzig selector), orthogonal decomposition (Singular Value Decomposition Principal Regression Method; SVDPRM) and model averaging.

Forward selection

This procedure starts with the null model and adds the most significant factor main effect at each step according to an F-test (Miller, 2002, pp. 39-42). The process continues until the model is saturated or no further factors are significant. The evidence required for the entry of a variable is controlled by the "F-to-enter" level, denoted by $\alpha \in (0, 1)$.

Gauss-Dantzig selector

Shrinkage methods form a class of continuous variable selection techniques where each coefficient β_i is shrunk towards zero at a different rate. We investigate the Dantzig selector, proposed by Candes and Tao (2007), in which the estimator $\hat{\boldsymbol{\beta}}$ is the solution to

$$\min_{\hat{\boldsymbol{\beta}} \in \mathbb{R}^k} ||\hat{\boldsymbol{\beta}}||_1 \quad \text{subject to} \quad ||\mathbf{X}^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})||_\infty \leq \delta \,. \tag{2.4}$$

Here $||\boldsymbol{\beta}||_1 = |\beta_0| + \ldots + |\beta_m|$ is the l_1 norm, $||\boldsymbol{a}||_\infty = \max(|a_0|, \ldots, |a_m|)$ is the l_∞ norm, and δ is a tuning constant. The Dantzig selector essentially finds the most parsimonious estimator amongst all those that agree with the data. Optimisation (2.4) may be reformulated as a linear program and solved, for example, using the package `lpSolve` (Berkelaar, 2007) in `R` (R Development Core Team, 2009).

Candes and Tao (2007) also developed a two-stage estimation approach, the Gauss-Dantzig selector, which reduces underestimation bias and was used for the analysis of supersaturated designs by Phoa et al. (2009). First the Dantzig selector is used to identify the active factors, and those factors whose coefficient estimates are greater than γ are retained. Second, least-squares estimates are found by regressing the response on the set of retained factors.

Singular Value Decomposition Principal Regression Method (SVDPRM)

Georgiou (2008) introduced the SVDPRM, based on an orthogonal decomposition of a subset of the factor columns in $\mathbf{X}$. The method has the following steps:

1. Retain the $\lfloor n/2 \rfloor$ factors with the largest absolute standardised contrasts and use them to form a reduced model matrix $\mathbf{X}_r$, where $\lfloor a \rfloor$ is the largest integer below a.

2. Calculate the singular value decomposition of $\mathbf{X}_r$:

$$\mathbf{X}_r = \mathbf{U}_r \mathbf{D}_r \mathbf{V}_r^T ,$$

   where $\mathbf{X}_r$ is an $n \times (\lfloor n/2 \rfloor + 1)$ matrix of rank t, $\mathbf{U}_r$ is an $n \times n$ orthogonal matrix, $\mathbf{V}_r$ is an $(\lfloor n/2 \rfloor + 1) \times (\lfloor n/2 \rfloor + 1)$ orthonormal matrix, and $\mathbf{D}_r$ is an $n \times (\lfloor n/2 \rfloor + 1)$ matrix containing the singular values. Dropping rows and columns corresponding to zero singular values gives

$$\mathbf{X}_t = \mathbf{U}_t \mathbf{D}_t \mathbf{V}_t^T ,$$

   where $\mathbf{X}_t$, $\mathbf{U}_t$, $\mathbf{D}_t$ and $\mathbf{V}_t$ are square $t \times t$ matrices and the columns of $\mathbf{U}_t$ are the t left singular vectors.

3. Fit a linear main effects regression model with the t left singular vectors as factors.

4. Transform the obtained coefficients back to the original variables and perform F-tests to establish which are active.

By fitting a model in the orthogonal left singular vectors, we hope to obtain coefficients with smaller bias. Notice that this method can identify at most $\lfloor n/2 \rfloor$ active factors. However, this is in line with the assumption of effect sparsity.

Model averaging

Here inference is based on a subset of models rather than on a single model. For example, model-averaged coefficients are obtained by calculating estimates for a set of models and then computing a weighted average where the weights represent the plausibility of each model (Burnham and Anderson, 2002, ch. 4). This approach provides more stable inference under repeated sampling from the same process.

For a supersaturated design, it is often not computationally feasible to include all possible models in the procedure. Further, many models will be scientifically implausible and therefore should be excluded (Madigan and Raftery, 1994). Effect sparsity suggests restriction to a set of models each of which contains only a few factors. We propose a new iterative approach, motivated by the *many-models* method of Holcomb et al. (2007).

1. Fit all models composed of two factors and the intercept and calculate for each the value of the Bayesian Information Criterion (BIC)

$$BIC = n \log\Big(\frac{(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n}\Big) + p \log(n)\,, \tag{2.5}$$

   where p is the number of model terms.

2. For model i, calculate a weight

$$w_i = \frac{\exp(-0.5 \times \Delta BIC_i)}{\sum_{k=1}^{K} \exp(-0.5 \times \Delta BIC_k)}\,, \qquad i = 1, \ldots, K\,,$$

   where $\Delta BIC_i = BIC_i - \min_{1,\ldots,K}(BIC_k)$ and $K = m(m-1)/2$.

3. For each factor, sum the weights of those models containing the factor. Retain the $m_1 < m$ factors with the highest summed weights. Parameter m_1 should be set fairly high to avoid discarding active factors.

4. Fit all possible models composed of three of the m_1 factors and the intercept. Calculate weights as in step 2. Retain the best $m_2 < m_1$ factors, as in step 3, to eliminate models of low weight and obtain more reliable inference.

5. Fit all M models composed of $m_3 < m_2$ factors and the intercept, where $M = m_2!/m_3!(m_2 - m_3)!$. Calculate new weights as in step 2.

6. Let $\beta^{\star}_{1r}, \ldots, \beta^{\star}_{m_2 r}$ be the coefficients of the m_2 factors in the rth model ($r = 1, \ldots, M$), where we set $\beta^{\star}_{lr} = 0$ if the lth factor is not included in model r. Calculate model-averaged coefficient estimates

$$\bar{\beta}_l^\star = \sum_{r=1}^{M} w_r \hat{\beta}_{lr}^\star \,,$$

where $\hat{\beta}_{lr}^\star$ is the least-squares estimate of $\beta_{lr}^\star$ if factor l is in model r, and 0 otherwise.

7. Use an approximate t-test, on $n - m_3 - 1$ degrees of freedom, to decide if each of the m_2 factors is active. The test statistic is given by $\bar{\beta}_l^\star / \{\widehat{\mathrm{Var}}(\bar{\beta}_l^\star)\}^{1/2}$, where estimation of the model-averaged variance is given by

$$\widehat{\mathrm{Var}}(\bar{\beta}_l^\star) = \left[\sum_{r=1}^{M} w_r \sqrt{\widehat{\mathrm{Var}}(\hat{\beta}_{lr}^\star) + (\hat{\beta}_{lr}^\star - \bar{\beta}_l^\star)^2} \right]^2 ,$$

and is discussed by Burnham and Anderson (2002, pp. 158-164).

The effectiveness of the each of the three methods described above depends on the values chosen for the tuning constants, discussed in Section 2.3.3.

2.3 Simulation Study and Results

We identified a variety of features of a typical screening experiment and combined these to provide settings of varying difficulty on which to test the design and model selection methods.

2.3.1 Features varied in the simulation

- *Ratio of factors to runs in the experiment.* Three choices of increasing difficulty were used and coded m_n: 22 factors in 18 runs (22_18), 24 in 14 (24_14) and 26 in 12 (26_12).

- *Design construction criteria.* To investigate the use of $E(s^2)$-optimal and Bayesian D-optimal designs, one design was found for each m_n under each criterion. These designs were then used for all simulations with m factors and n runs. For each design, the values of the objective functions $E(s^2)$ and ϕ_D are

given in Table 2.1, together with the maximum (ρ_{max}) and minimum (ρ_{min}) correlations between factor columns.

For each m_n, the designs have similar values of $E(s^2)$ and ϕ_D but different structures. The $E(s^2)$-optimal designs are balanced, whereas the Bayesian D-optimal designs have 9, 7, and 5 unbalanced columns for the 22_18, 24_14 and 26_12 experiments respectively, with column sums of ± 2. Also, the Bayesian D-optimal designs have a wider range of column correlations than the $E(s^2)$-optimal designs. In particular, ρ_{max} for an $E(s^2)$-optimal design is always less than or equal to that of the corresponding Bayesian D-optimal design.

- *Number and sizes of active factors.* The magnitude of the coefficient for each of the c active factors was drawn at random from a $N(\mu, 0.2)$ for the following scenarios.

  1. Effect sparsity: $c = 3$, $\mu = 5$.
  2. Intermediate complexity: $c = 4$ or $c = 5$ (chosen with equal probability) and $\mu = 4$.
  3. Larger number of small effects: $c = 6$ and $\mu = 3$.
  4. Larger number of effects of mixed size: $c = 9$ and one factor with each of $\mu = 10$, $\mu = 8$, $\mu = 5$, $\mu = 3$, and five factors with $\mu = 2$.

- *Model selection methods.* The four methods of Section 2.2.2 were applied and tuning constants chosen as described in Section 2.3.3.

Table 2.1: Values of objective functions and maximum and minimum column correlations for $E(s^2)$-optimal and Bayesian D-optimal designs used in the simulation study

Experiment	22_18		24_14		26_12	
Construction Criterion	$E(s^2)$	D	$E(s^2)$	D	$E(s^2)$	D
$E(s^2)$	5.3	5.4	7.2	7.1	7.5	7.3
ϕ_D	11.7	11.7	6.1	6.1	4.3	4.3
ρ_{max}	0.33	0.33	0.43	0.58	0.33	0.67
ρ_{min}	0.11	0	0.14	0	0	0

2.3.2 Experiment simulation

For each of 10,000 iterations:

1. From columns $2, \ldots, m+1$ of $\mathbf{X}$, c columns were assigned to active factors at random.

2. To obtain the coefficients for the active factors, a sample of size c was drawn from a $N(\mu, 0.2)$, and $\pm$ signs randomly allocated to each number.

3. Coefficients for the inactive factors were obtained as a random draw from a $N(0, 0.2)$.

4. Data were generated from model (2.1), with errors randomly drawn from a $N(0, 1)$, and analysed by each of the four model selection methods.

The random assignment of active factors to columns is important to remove selection bias. The choice of distributions at steps 2 and 3 ensures separation between the realised coefficients of the active and inactive factors.

2.3.3 Choice of tuning constants

For each method, a comparison of different values for the tuning constants was carried out prior to the main simulation studies. The aim was to find values of the tuning parameters that did not rely on detailed information from each simulation setting. This was achieved either by choosing values to give robust performance across the different settings, or by applying automated adaptive procedures.

Our strategy for the selection of δ and γ for the Gauss-Dantzig selector was to control type II errors via δ, by choosing a larger than necessary model with the Dantzig selector, and then control type I errors by choosing γ sufficiently large to screen for spurious effects. To choose δ we used the standard BIC statistic (2.5) which gave similar results to the use of AIC. Phoa et al. (2009) proposed a modified AIC criterion which, in our study, consistently selected too few active effects when $c = 6$. The value of γ needs to be sufficiently small so that few active factors are declared inactive, but large enough for effects retained by the Dantzig selector to

be distinguishable from the random error. This was achieved by the choice $\gamma = 1.5$. For Scenario 4, with $\mu = 2$, an active effect may occasionally have magnitude less than γ, resulting in slightly conservative results for the Gauss-Dantzig selector.

Model averaging is the most computationally demanding of the methods due to the large number of regression models fitted. In the choice of m_1, m_2 and m_3, a balance must be struck between discarding potentially active factors too early in the procedure, and including unlikely (for example, too large) models in the final step. Preliminary studies showed that $m_1 = 18$, $m_2 = 13$ and $m_3 = 8$ was an effective compromise. In step 5 of the procedure, some models may not be estimable. We found that removing a single factor overcame this problem. We therefore chose to remove the factor with smallest weight that produced a non-singular information matrix. Reassuringly, the power of the procedure to detect active effects (see Section 2.3.4) is relatively robust to the values of m_1 and m_2. Attempting to fit too large models in step 5, i.e. setting m_3 too high, can result in loss of power and also higher type I errors. We suggest that m_3 is chosen broadly in line with effect sparsity, and a little larger than the anticipated number of active factors.

In forward selection, SVDPRM and model averaging, $\alpha = 0.05$ was used based on investigations (not presented) that showed $\alpha > 0.05$ gave a substantial increase in type I errors without a corresponding increase in power. Decreasing α resulted in unacceptably low power for even the easiest simulation settings.

For each method studied, the results of the analysis can depend critically on the choice of tuning constants. The Gauss-Dantzig selector has the advantages of having a robust automated procedure for the choice of δ, and a straightforward interpretation of γ as the minimum size of an active effect considered important enough to detect. This quantity may often be elicited from subject experts (see, for example, Δ, in Lewis and Dean, 2001).

2.3.4 Simulation results

A factorial set of 96 simulations was run on the four features of Section 2.3.1. Four different criteria were used to assess performance of the designs and analysis meth-

Table 2.2: Simulation study results for 22_18 designs. FS=forward selection, GDS=Gauss-Dantzig selector, SVD=SVDPRM, MA=model averaging; π_1=power, π_2=type I error rate, π_3=coverage, π_4=number of factors declared active

Design	$E(s^2)$-optimal				Bayesian D-optimal			
Analysis	FS	GDS	SVD	MA	FS	GDS	SVD	MA
Scenario 1: $c = 3$, $\mu = 5$								
π_1	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
π_2	0.11	0.01	0.05	0.02	0.11	0.03	0.05	0.02
π_3	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
π_4	5.07	3.17	3.99	3.41	5.07	3.61	3.97	3.42
Scenario 2: $c = 4$ or $c = 5$, $\mu = 4$								
π_1	0.89	1.00	0.97	0.99	0.90	1.00	0.97	0.99
π_2	0.09	0.01	0.04	0.02	0.10	0.04	0.04	0.02
π_3	0.85	0.99	0.92	0.98	0.86	0.99	0.92	0.98
π_4	5.57	4.72	5.06	4.74	5.69	5.11	5.04	4.74
Scenario 3: $c = 6$, $\mu = 3$								
π_1	0.57	0.93	0.86	0.90	0.58	0.95	0.86	0.89
π_2	0.06	0.02	0.03	0.02	0.06	0.04	0.03	0.02
π_3	0.37	0.77	0.60	0.74	0.38	0.82	0.60	0.73
π_4	4.35	5.97	5.68	5.63	4.43	6.26	5.68	5.62
Scenario 4: $c = 9$, $\mu = 10, 8, 5, 3, 2$								
π_1	0.56	0.73	0.47	0.55	0.56	0.75	0.47	0.56
$\pi_1(10, 8)$	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
$\pi_1(5, 3)$	0.78	0.92	0.64	0.80	0.78	0.93	0.64	0.80
$\pi_1(2)$	0.30	0.55	0.19	0.28	0.30	0.58	0.18	0.28
π_2	0.04	0.06	0.03	0.02	0.05	0.07	0.03	0.02
π_3	0.04	0.08	0.00	0.00	0.05	0.10	0.00	0.00
π_4	5.63	7.37	4.57	5.22	5.64	7.73	4.54	5.24

ods.

π_1: Average proportion of active factors correctly identified (Power; larger-the-better); for Scenario 4, the power was calculated separately for effects with $\mu = 10, 8$ (dominant; $\pi_1(10, 8)$), $\mu = 5, 3$ (moderate; $\pi_1(5, 3)$) and $\mu = 2$ (small; $\pi_1(2)$).

π_2: Average proportion of inactive factors which are declared active (Type I error rate; smaller-the-better).

π_3: Average proportion of simulations in which the set of factors declared active included all those truly active (Coverage; larger-the-better).

Table 2.3: Simulation study results for 24_14 designs. FS=forward selection, GDS=Gauss-Dantzig selector, SVD=SVDPRM, MA=model averaging; π_1=power, π_2=type I error rate, π_3=coverage, π_4=number of factors declared active

Design	$E(s^2)$-optimal				Bayesian D-optimal			
Analysis	FS	GDS	SVD	MA	FS	GDS	SVD	MA
Scenario 1: $c = 3$, $\mu = 5$								
π_1	0.86	0.98	0.93	0.91	0.86	0.99	0.93	0.90
π_2	0.11	0.03	0.03	0.05	0.11	0.04	0.03	0.05
π_3	0.82	0.97	0.87	0.84	0.82	0.98	0.87	0.81
π_4	4.77	3.54	3.33	3.83	4.81	3.75	3.36	3.83
Scenario 2: $c = 4$ or $c = 5$, $\mu = 4$								
π_1	0.53	0.85	0.64	0.73	0.53	0.89	0.65	0.72
π_2	0.09	0.06	0.03	0.06	0.09	0.07	0.03	0.06
π_3	0.31	0.69	0.37	0.50	0.31	0.76	0.38	0.48
π_4	4.03	5.04	3.35	4.47	4.02	5.25	3.42	4.45
Scenario 3: $c = 6$, $\mu = 3$								
π_1	0.31	0.61	0.38	0.46	0.30	0.65	0.40	0.46
π_2	0.08	0.09	0.03	0.09	0.08	0.09	0.03	0.09
π_3	0.02	0.20	0.04	0.11	0.02	0.26	0.05	0.10
π_4	3.22	5.23	2.84	4.29	3.16	5.57	2.93	4.31
Scenario 4: $c = 9$, $\mu = 10, 8, 5, 3, 2$								
π_1	0.40	0.53	0.30	0.40	0.40	0.56	0.30	0.39
$\pi_1(10, 8)$	0.90	0.98	0.90	0.90	0.91	0.99	0.91	0.88
$\pi_1(5, 3)$	0.47	0.65	0.28	0.45	0.49	0.69	0.28	0.45
$\pi_1(2)$	0.16	0.31	0.07	0.18	0.16	0.33	0.07	0.18
π_2	0.08	0.14	0.03	0.09	0.08	0.14	0.03	0.09
π_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
π_4	4.76	6.89	3.07	4.86	4.74	7.14	3.13	4.86

π_4: Average number of declared active factors.

The results are summarised in Tables 2.2, 2.3 and 2.4 for experiments 22_18, 24_14 and 26_12 respectively. These show that the Gauss-Dantzig selector has values of π_1 and π_3 as high, or higher, than the other analysis methods in almost all the simulations and often has very low values for π_2. The Gauss-Dantzig selector was found to have the most consistent performance of the three methods as measured by the variances (not shown) of the proportions involved in π_1, π_2 and π_3.

For the 22_18 experiment (Table 2.2), the performance of the Gauss-Dantzig selector is almost matched by the model-averaging method for Scenarios 1–3. However, the

Table 2.4: Simulation study results for 26_12 designs. FS=forward selection, GDS=Gauss-Dantzig selector, SVD=SVDPRM, MA=model averaging; π_1=power, π_2=type I error rate, π_3=coverage, π_4=number of factors declared active

Design	$E(s^2)$-optimal				Bayesian D-optimal			
Analysis	FS	GDS	SVD	MA	FS	GDS	SVD	MA
Scenario 1: $c = 3$, $\mu = 5$								
π_1	0.66	0.89	0.70	0.67	0.67	0.92	0.73	0.68
π_2	0.11	0.06	0.02	0.09	0.11	0.06	0.02	0.10
π_3	0.54	0.82	0.56	0.48	0.56	0.87	0.60	0.47
π_4	4.43	3.95	2.60	4.14	4.44	4.10	2.70	4.36
Scenario 2: $c = 4$ or $c = 5$, $\mu = 4$								
π_1	0.37	0.65	0.37	0.45	0.36	0.69	0.37	0.47
π_2	0.10	0.10	0.03	0.11	0.10	0.10	0.03	0.12
π_3	0.10	0.35	0.12	0.15	0.09	0.41	0.11	0.15
π_4	3.71	5.00	2.15	4.36	3.63	5.22	2.21	4.62
Scenario 3: $c = 6$, $\mu = 3$								
π_1	0.25	0.43	0.21	0.31	0.25	0.47	0.22	0.32
π_2	0.10	0.11	0.03	0.12	0.09	0.11	0.03	0.13
π_3	0.00	0.04	0.00	0.01	0.00	0.07	0.00	0.01
π_4	3.47	4.71	1.85	4.31	3.36	5.00	1.90	4.46
Scenario 4: $c = 9$, $\mu = 10, 8, 5, 3, 2$								
π_1	0.31	0.44	0.22	0.31	0.31	0.47	0.22	0.32
$\pi_1(10, 8)$	0.75	0.93	0.72	0.68	0.75	0.94	0.73	0.69
$\pi_1(5, 3)$	0.31	0.48	0.15	0.31	0.31	0.52	0.16	0.32
$\pi_1(2)$	0.14	0.23	0.04	0.16	0.14	0.25	0.04	0.17
π_2	0.10	0.15	0.02	0.12	0.10	0.15	0.02	0.13
π_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
π_4	4.48	6.56	2.32	4.83	4.45	6.78	2.39	5.04

good performance of model averaging is not maintained for the more difficult 24_14 and 26_12 experiments. The addition of extra steps in the procedure, such as fitting all four-factor models, may improve performance for larger numbers of factors at the cost of more computation.

Forward selection has consistently the worst performance for Scenarios 1–3 measured by π_1 and π_3, and also performs poorly under π_2 for $c = 3$ and $c = 4, 5$. Also, the type I error rate (π_2) is often higher than the value set for the entry of a variable, $\alpha = 0.05$, due to the multiple testing. SVDPRM performs badly for Scenario 4, which has a particularly large number of active factors. This poor performance is, in part, due to the method being able to select at most $\lfloor n/2 \rfloor$ active factors.

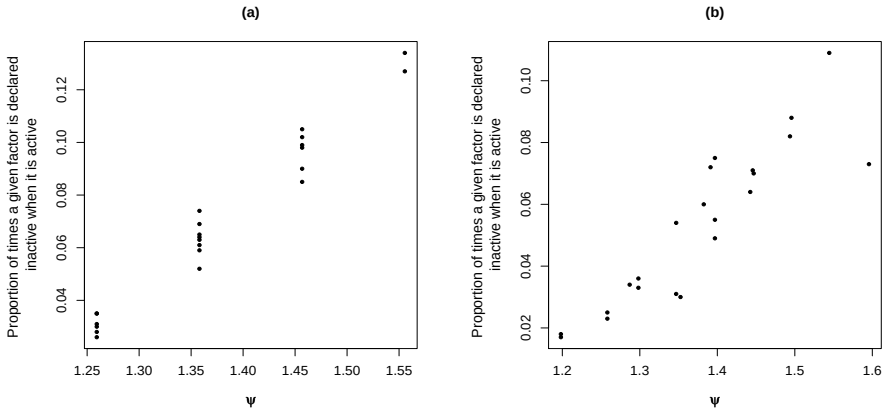


Figure 2.1: Proportion of times a given factor was wrongly declared inactive plotted against ψ, for the 22_18 experiment and Scenario 3 analysed using the Gauss-Dantzig selector: (a) $E(s^2)$-optimal design; (b) Bayesian D-optimal design.

From our comparisons, the Gauss-Dantzig selector is the most promising method, particularly in the more challenging settings. For example, for the 26_12 experiment with $c = 3$, $\mu = 5$ (Table 2.4), the Gauss-Dantzig selector has a 26% increase in power (π_1) and a 45% increase in coverage (π_3), relative to the next best method (SVDPRM). In Scenario 4 for the 26_12 experiment, the Gauss-Dantzig selector performs extremely well in identifying the dominant factors ($\mu = 8$, $\mu = 10$), having $\pi_1 > 0.93$; the next best method (forward selection) has $\pi_1 = 0.75$. All methods had difficulty identifying small active effects; reducing γ in the Gauss-Dantzig selector may improve performance for this situation, at the cost of a higher type I error rate.

To compare the supersaturated designs, we now focus on the preferred analysis via the Gauss-Dantzig selector. The Bayesian D-optimal designs have consistently higher values for $\pi_1, \ldots, \pi_4$ than the $E(s^2)$-optimal designs, although the differences are often small. Thus the Bayesian D-optimal designs lead to identifying as active a slightly higher proportion of both active and inactive effects. All designs give their best results for Scenario 1 and the worst for Scenarios 3 and 4, as expected. Performance deteriorates as the ratio of factors to runs increases, although good results are obtained under Scenario 1 (effect sparsity) for all m_n.

When there are few active factors in the 26_12 experiment, both classes of designs performed well under effect sparsity (Scenario 1, Table 2.4). To investigate if performance is maintained when the number of factors is increased substantially, simu-

lations of a 48_12 experiment were performed using each type of design. The results indicated poor performance with π_1 and π_3 less than 0.61 and 0.37 respectively.

In practice, the assignment of active factors to the columns of a design may influence the subsequent model selection. This was investigated by measuring the overall level of correlation of a given column j of $\mathbf{X}$ by

$$\psi_j = \sum_{i=2}^{m+1} \rho_{ij}^2 \,,$$

where ρ_{ij} is the correlation between columns i and j of $\mathbf{X}$ $(i, j = 2, \ldots, m+1)$. Fig. 2.1 shows the proportion of times that a given factor was wrongly declared inactive as a function of ψ for the 22_18 experiment and $c = 6$, $\mu = 3$, analysed using the Gauss-Dantzig selector. There are strong positive correlations for both the $E(s^2)$-optimal and Bayesian D-optimal designs, 0.98 and 0.90 respectively. Similar trends were observed for other simulated experiments and scenarios (not shown). This demonstrates the importance of using any prior information on the likely activity of factors when assigning them to columns of the design. For the Bayesian D-optimal design, any such information should ideally be incorporated in the design construction through adjusting the elements of the matrix $\mathbf{K}$ in (2.3).

2.3.5 No active factors

Further simulations were used to check the performance of the design and analysis methods when there are no active factors, a situation where π_1 (power) and π_3 (coverage) no longer apply. From Table 2.5, the Gauss-Dantzig selector is clearly the best analysis method and rarely declares any factors active. The other methods have considerably higher type I errors, typically declaring at least two factors active. Table 2.5 also shows that the $E(s^2)$-optimal designs perform better than the Bayesian D-optimal designs for the Gauss-Dantzig selector, agreeing with the results for π_2 in Section 2.3.4.

Table 2.5: Simulation results when there were no active factors. FS=forward selection, GDS=Gauss-Dantzig selector, SVD=SVDPRM, MA=model averaging; π_2=type I error rate, π_4=number of factors declared active

Design	$E(s^2)$-optimal				Bayesian D-optimal			
Analysis	FS	GDS	SVD	MA	FS	GDS	SVD	MA
22_18								
π_2	0.11	0.01	0.19	0.05	0.12	0.03	0.19	0.05
π_4	2.52	0.12	4.15	1.13	2.55	0.57	4.11	1.14
24_14								
π_2	0.12	0.01	0.10	0.08	0.12	0.02	0.10	0.08
π_4	2.88	0.23	2.40	1.85	2.82	0.43	2.47	1.88
26_12								
π_2	0.13	0.01	0.07	0.10	0.12	0.02	0.07	0.11
π_4	3.28	0.33	1.74	2.64	3.22	0.52	1.81	2.83

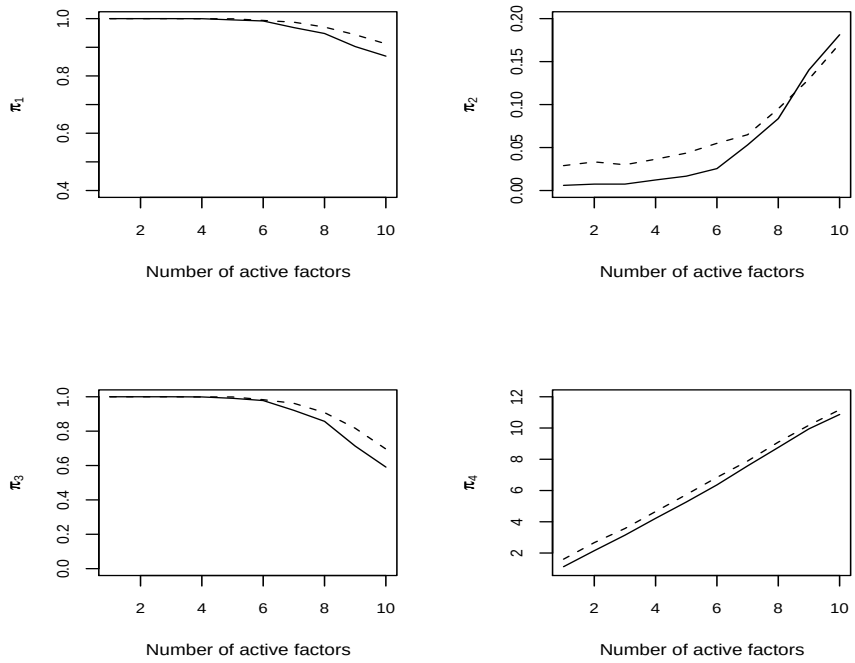


Figure 2.2: Performance measures, $\pi_1, \ldots, \pi_4$, for the 22_18 experiment with $\mu = 5$ using the Gauss-Dantzig selector for $E(s^2)$ (solid line) and Bayesian D-optimal (dashed line) designs.

2.3.6 What is 'effect sparsity'?

A set of simulations was performed to assess how many active factors could be identified reliably using supersaturated designs. These simulations kept the mean,

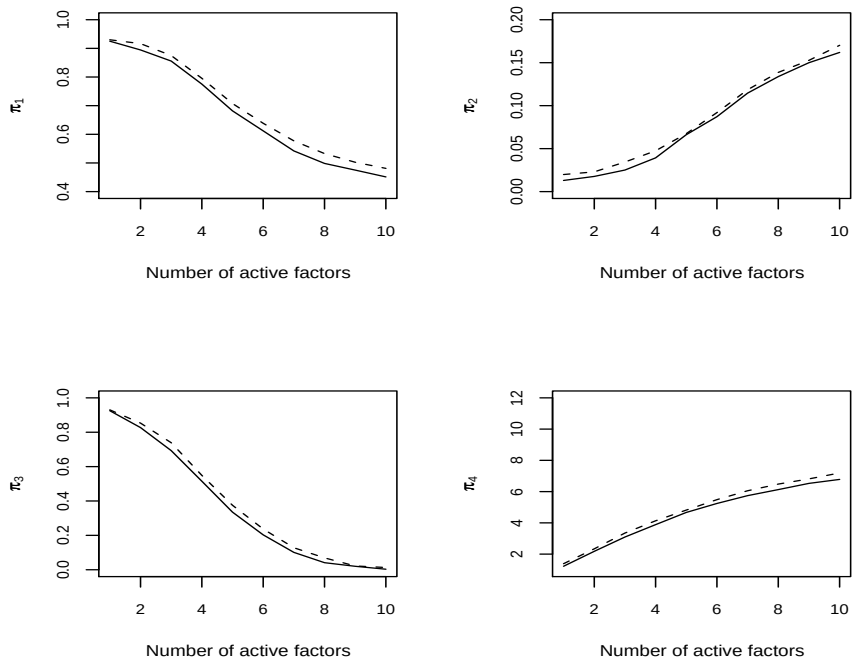


Figure 2.3: Performance measures, $\pi_1, \ldots, \pi_4$, for the 24_14 experiment with $\mu = 3$ using the Gauss-Dantzig selector for $E(s^2)$ (solid line) and Bayesian D-optimal (dashed line) designs.

μ, of an active factor constant and varied the number of active factors, $c = 1, \ldots, 10$. Fig. 2.2 shows the four performance measures for the 22_18 experiment with $\mu = 5$ using the Gauss-Dantzig selector for analysis. Both the $E(s^2)$-optimal and the Bayesian D-optimal designs perform well for up to eight active factors. The Bayesian D-optimal design has slightly higher π_1, π_2 and π_3 values and thus tends to select slightly larger models.

Fig. 2.3 shows the corresponding results for 24_14 experiment with $\mu = 3$. The performance, particularly under π_1 and π_3, declines more rapidly as the number of active factors increases. Again, slightly larger models are selected using the Bayesian D-optimal design, a difference which is not consistently observed for other analysis methods. Further simulations (not shown) indicate considerable differences in performance between settings where $\mu = 3$ and $\mu = 5$.

2.4 Discussion

The results in this chapter provide evidence that supersaturated designs may be a useful tool for screening experiments, particularly marginally supersaturated designs (where m is only slightly larger than n). They suggest the following guidelines for the use of supersaturated designs.

1. The Gauss-Dantzig selector is the preferred model selection procedure out of the methods investigated. If the design is only marginally supersaturated, model averaging is also effective.

2. The ratio of factors to runs should be less than 2.

3. The number of runs should be at least three times the anticipated number of active factors.

The simulations include situations where these conditions do not hold but nevertheless a supersaturated design performs well, for example, Table 2.4 Scenario 1 with $m/n > 2$. However, evidence from our study suggests that 2 and 3 are conditions under which supersaturated designs are most likely to be successful.

We notice that in Scenario 4 the assumption of effect sparsity is clearly violated, with there being very many small active effects. However, the Gauss-Dantzig selector is still very effective at picking out the largest effects.

With respect to guideline 3, we acknowledge that the experimenter will not know the true number of active factors before performing the experiment. However, we can use any available prior information about which factors may be active to guide the choice of experiment size.

Little difference was found in the performance of the $E(s^2)$-optimal and Bayesian D-optimal designs, with the latter having slightly higher power to detect active effects at the cost of a slightly higher type I error rate. The Bayesian D-optimal designs may be preferred in practice, despite being unbalanced and having some high column correlations, as follow-up experimentation may screen out spurious factors

but cannot detect active factors already removed. Such designs are readily available in standard software such as SAS Proc Optex and JMP.

The simulations presented cover a broader range of conditions than previously considered and investigate more aspects of design performance. Further studies of interest include incorporating interaction effects in the models, and Bayesian methods of analysis, see for example Beattie et al. (2002).

Chapter 3

Optimal supersaturated designs under measures of multicollinearity with application to experiments where combinations of factor levels cannot be set independently

Supersaturated designs may be defined as experimental plans with at least as many factors as runs. Most existing criteria for generating or assessing supersaturated designs focus only on dependencies between pairs of factors. We propose a new class of criteria for supersaturated designs based on measures of multicollinearity among subsets of the factors. Unlike some existing criteria, this new class can be used to design experiments where factor levels cannot be set independently. We apply the new criteria to two such experiments with a large list of possible design points to choose from. We also generate new two- and three-level supersaturated designs. The examples are used to demonstrate the benefits of the new methodology and to illustrate some desirable properties of the resulting designs.

3.1 Introduction

3.1.1 Background

When performing experiments, there is often pressure to keep the number of runs performed to a minimum, in order to reduce costs. In certain circumstances an experimenter may wish to use a supersaturated design (SSD). Such designs have more factors than runs. These designs are useful in screening situations, where the experimenter initially wishes to determine which factors are 'active' (that is have a large effect on the response of interest), rather than fitting a precise model. It is widely accepted that the success of these designs in detecting the factors which have a large impact on the response relies on the assumption of effect sparsity (Box and Meyer, 1986).

There is much work in the literature on how to design two-level supersaturated experiments. Booth and Cox (1962) proposed the popular $E(s^2)$ criterion, which involves making the columns of the design matrix as near orthogonal as possible. Lin (1993) proposed using half fractions of Hadamard matrices to construct SSDs, whilst Wu (1993) supplemented Hadamard matrices with interaction columns. Wu (1993) also briefly discussed A- and D-criteria which are extensions of classical design optimality criteria that average over different models. Deng et al. (1996) also discussed these ideas and proposed a new class of criteria, called B-optimality. Nguyen (1996) found designs via algorithmic search using the $E(s^2)$ criterion, whilst more recently Jones et al. (2008) used the coordinate exchange algorithm of Meyer and Nachtsheim (1995) to generate designs based on Bayesian D-optimality.

There has also been interest in multi-level supersaturated experiments. Yamada and Lin (1999) proposed the χ^2 criterion and gave a construction method for three-level SSDs. Chen and Liu (2008) and Liu and Lin (2009) proposed further methods for constructing χ^2-optimal mixed-level SSDs. Xu and Wu (2005) proposed the generalised minimum aberration criterion for multi-level SSDs.

Most of the existing design criteria involve minimising dependencies between *pairs* of columns. However, in even moderate sized experiments, it is quite possible that there are more than two active factors. In order to achieve good projection properties

for the active factors, it is necessary to consider linear dependencies among more than two factors. In this chapter we propose a new set of criteria incorporating multicollinearity, and use this to generate two-level and multi-level designs.

Although there is much attention given to two-level and multi-level SSDs, there is little work on cases where the levels of the factors cannot be set independently. Such cases often occur in experimentation involving chemical compounds (see for instance Put et al., 2004). The experimenter has a list of compounds which have different properties. In this case, the properties are the factors in the experiment and one compound must be chosen for each run of the experiment. Clearly, choosing the compound fixes the levels of all the factors for this run and we have a different design problem to the standard two-level or multi-level situation. We apply our new set of criteria to such experiments and illustrate how its implementation can result in designs with desirable properties.

Marley and Woods (2010) showed that, in practice, the choice of columns of the design to which the active factors are assigned may have an impact on the power to detect them. Xu and Wu (2005) suggested some designs with one column orthogonal to the rest, which can be useful if the experimenter believes one particular factor is very likely to be active. More generally, Li et al. (2010) proposed a cluster based method for assigning factors to columns when some prior information is available. The current chapter provides a new method of factor to column assignment and demonstrates its affect in existing Bayesian D-optimal and $E(s^2)$-optimal supersaturated designs.

The remainder of this chapter is organised as follows. In Section 3.1.2 we review the concept of variance inflation factors (VIFs) for SSDs and propose a set of new criteria for use in evaluating existing designs. In Section 3.2 we consider assignment of factors to columns. Section 3.3 details a VIF based set of criteria which can be used to generate new SSDs. Section 3.4 considers generating two-level and three-level SSDs using the VIF based criterion to minimise multi-factor collinearity, whilst Section 3.5 generates SSDs for cases where factor levels cannot be set independently. Some discussion and concluding remarks are presented in Section 3.6.

3.1.2 Design selection criteria

Crosier (2000) stated that the multicollinearity of a set of variables cannot be established from only their pairwise correlations. With supersaturated designs, the aliasing schemes are often very complex, with factorial effects normally partially aliased with several other effects. With this in mind, it makes sense to consider dependencies amongst linear combinations of factors in the design and try to minimise the impact of such relationships on the power to identify active factors.

Let $\mathbf{X}$ be a $n \times m$ design matrix. The (hj)th entry of $\mathbf{X}$ represents the level of factor j for run h. One way of quantifying the linear dependencies amongst more than two columns is to look at the variance inflation factors of $\mathbf{X}$.

Consider first the non-supersaturated case. Then the variance inflation factor for the kth variable $(k = 1, \ldots, m)$ is defined as

$$\nu_k = (1 - R_k^2)^{-1} \,,$$

where R_k^2 is the R^2 statistic when column k is regressed on all the other columns of $\mathbf{X}$ and the intercept, that is

$$R^2 = SS_{reg}/SS_{tot} \,,$$

where SS_{reg} and SS_{tot} are respectively the regression sum of squares and the total sum of squares from a regression of column k on all other columns.

The ν_k $(k = 1, \ldots, m)$ can be interpreted as how much the variance of the kth estimated regression coefficient is inflated as compared to when the columns of $\mathbf{X}$ are not linearly related. Clearly lower VIFs imply less linear dependence among columns in the design matrix.

Let ρ_{ij} be the correlation between column i and column j of $\mathbf{X}$ and let the correlation matrix for a given $\mathbf{X}$ be denoted by $\boldsymbol{\rho} = (\rho_{ij})$. Then

Result 1: The VIFs of a design can be expressed as the diagonal elements of the inverse of the correlation matrix $\boldsymbol{\rho}$ (Neter et al., 1996, pp. 386).

Further, let $\tilde{\boldsymbol{X}}$ be the standardised design matrix (formed by columnwise subtraction of the mean and dividing by the column standard deviation). Then

Result 2: The $\sum_{k=1}^{m} \nu_k$ can be expressed in terms of eigenvalues of the information matrix formed from the standardised design matrix $\tilde{\boldsymbol{X}}$.

This can be shown as follows. The correlation matrix is $\boldsymbol{\rho} = \tilde{\boldsymbol{X}}'\tilde{\boldsymbol{X}}/n$ and the ν_k are the diagonal elements of the inverse of the correlation matrix. So

$$\sum_{k=1}^{m} \nu_k = tr\left(\left(\frac{\tilde{\boldsymbol{X}}'\tilde{\boldsymbol{X}}}{n}\right)^{-1}\right) = ntr((\tilde{\boldsymbol{X}}'\tilde{\boldsymbol{X}})^{-1})$$

Note that if $\mathbf{A}$ is an $n \times n$ symmetric matrix with r non-zero eigenvalues $\lambda_1, \ldots, \lambda_r$ then $tr(\mathbf{A}^-) = \sum_{i=1}^{r} \lambda_i^{-1}$.

Hence

$$\sum_{k=1}^{m} \nu_k = n \sum_{k=1}^{m} \lambda_k^{-1},$$

where the λ_k are the eigenvalues of $\tilde{\boldsymbol{X}}'\tilde{\boldsymbol{X}}$.

Suppose that we calculate VIFs for subsets of size c of the columns in a given design. For a given subset of columns, $\mathcal{S}$, the variance inflation factor for the kth column in the set $\mathcal{S}$ is then

$$\nu_k(\mathcal{S}) = (1 - R^2(k, \mathcal{S}))^{-1}, \tag{3.1}$$

where $R^2(k, \mathcal{S})$ is the R^2 statistic when column k is regressed on all the other columns in $\mathcal{S}$ and the intercept.

Under the assumption of effect sparsity, it is likely that only a small subset of the factors in the experiment will be active. Therefore, it is desirable to have dependencies among this subset of factors as low as possible to give good projection properties of the design (i.e. the ability to estimate efficiently models containing a subset of the factors), see for example Lin (1993). Hence $\nu_k(\mathcal{S})$ could prove a useful tool for comparing existing SSDs or in a criterion for constructing new SSDs. An advantage of using variance inflation factors is that not only pairwise dependencies are evaluated, but also linear relationships involving more than two factors.

We initially propose two criteria for assessing and selecting designs. When evaluating a design based on $\nu_k(\mathcal{S})$, we can calculate the average of the $\nu_k(\mathcal{S})$ across all subsets of columns of size c, that is

$$\text{Criterion 1:} \qquad minimise \quad \bar{\nu}(c) = \frac{1}{cm'} \sum_{l=1}^{m'} \sum_{k=1}^{c} \nu_k(\mathcal{S}_l)\,,$$

where $\mathcal{S}_l$ is the lth subset of columns of size c ($l = 1, \ldots, m'$) and $m' = m!/c!(m-c)!$.

Similarly, we could also consider the maximum $\nu_k(\mathcal{S})$ of a design.

$$\text{Criterion 2:} \qquad minimise \quad \tilde{\nu}(c) = \max_{l=1,\ldots,m';\ k=1,\ldots,c} \nu_k(\mathcal{S}_l)$$

The idea of averaging $\nu_k(\mathcal{S})$ across different subsets is similar in principal to a set of criteria proposed by Deng et al. (1996). They stated that there is a problem with the widely used $E(s^2)$ criterion in that it provides no measurement of multi-factor orthogonality. They proposed a new set of criteria, based on the regression sum of squares, called B-optimality to deal with this problem, concentrating on producing near orthogonal projections onto the set of (possibly greater than two) active factors. The function they proposed is

$$V_c(\mathbf{X}) = \frac{1}{m'} \sum_{|\mathcal{S}|=c} v_g(\mathbf{X}_\mathcal{S})\,,$$

where

$$v_g(\mathbf{X}_\mathcal{S}) = \sum_{k \in \mathcal{S}} \beta'_{\mathcal{S}-k} (\mathbf{X}'_{\mathcal{S}-k} \mathbf{X}_{\mathcal{S}-k})^g \beta_{\mathcal{S}-k}\,.$$

$\mathbf{X}_\mathcal{S}$ is a $n \times c$ sub-matrix of design matrix $\mathbf{X}$, $\mathbf{X}_{\mathcal{S}-k}$ is a $n \times (c-1)$ matrix corresponding to $\mathcal{S}$ without k, $\mathbf{x}_k$ is a column corresponding to the kth unit in $\mathcal{S}$ and $\beta_{\mathcal{S}-k} = (\mathbf{X}'_{\mathcal{S}-k}\mathbf{X}_{\mathcal{S}-k})^{-1}\mathbf{X}'_{\mathcal{S}-k}\mathbf{x}_k$.

They consider the cases $g = 2, 1, 0$ to give different penalties on near singularity. The B_1 criterion (where $g = 1$) is equivalent to Criterion 1 for two-level balanced

designs. Deng et al. (1996) only used the B-criteria to assess existing designs, and did not generate any new designs.

3.2 Using measures of multicollinearity to assign factors to columns in existing designs

We now show how measures of multicollinearity can be used to aid the assignment of factors to columns within the designs. Marley and Woods (2010) show that the assignment of active factors to columns of the design could greatly influence the power to detect them in the analysis. If some prior information is available about which factors are more likely to be active, then we may wish to assign these factors to 'good' columns of the design, so that we are less likely to miss them.

Here we consider ranking columns of a design in order of their average VIFs. We define the average VIF for column f based on subsets of size c as

$$\bar{\nu}_f(c) = \frac{1}{\frac{cm'}{m}} \sum_{l=1}^{\frac{cm'}{m}} \nu_f(\mathcal{S}_l)\,,$$

where $\mathcal{S}_l$ is the lth subset of columns of size c which contain column f; $l = 1, \ldots, \frac{cm'}{m}$, and $\nu_f(\mathcal{S}_l)$ is defined in equation (3.1).

The ranking of the columns may change depending on the value of c. We recommend ranking with $c = n/3$. This is in line with a guideline proposed by Marley and Woods (2010), who demonstrated that when using a two-level SSD, an experimenter could reasonably expect to be able to detect up to $n/3$ active factors. They also showed that performance of SSDs was much better when there were a smaller number of active factors. Hence, ranking with $c = n/3$ corresponds to assigning factors to columns based on a worst-case scenario in terms of the number of active factors that might reasonably be detected. We consider assigning factors to columns in existing designs generated under two different criteria; $E(s^2)$-optimality and Bayesian D-optimality.

Nguyen (1996) used an algorithm to construct SSDs using the $E(s^2)$ criterion, which minimises the sum of the squared inner-products between columns i and j of $\mathbf{X}$

$(i, j = 1, \ldots, m)$.

$$E(s^2) = \frac{2}{m(m-1)} \sum_{i<j} s_{ij}^2 \,,$$

where s_{ij} is the ijth element of $\mathbf{X}'\mathbf{X}$. Notice how the $E(s^2)$ criterion only incorporates pairwise dependencies between the columns.

Jones et al. (2008) use Bayesian D-optimality as a criterion for generating SSDs. In the Bayesian approach, the prior information can be viewed as equating to extra runs in the experiment. Model uncertainty is incorporated through the choice of prior. The parameter τ^2 reflects how much prior information we have. The aim is to choose $\mathbf{X}$ to maximise

$$\phi_D = |[\mathbf{1}|\mathbf{X}]'[\mathbf{1}|\mathbf{X}] + \mathbf{K}/\tau^2| \,, \tag{3.2}$$

where $\mathbf{1}$ is a column of 1s and $\mathbf{K}$ is the prior dispersion matrix:

$$\mathbf{K} = \begin{pmatrix} 0 & \mathbf{0}_{1\times m} \\ \mathbf{0}_{m\times 1} & \mathbf{I}_{m\times m} \end{pmatrix} .$$

As an example of how designs can have very different average VIFs for different columns, Table 3.1 shows $\bar{\nu}_f(6)$ for all columns for Nguyen's $E(s^2)$-optimal design for 30 factors in 18 runs. We notice a 16% inflation in variance for column 10, which has the lowest average VIF, compared to a 28% inflation in variance for column 21, which has the highest.

To illustrate the difference in performance of this design and several others, when active factors are assigned to columns with low $\bar{\nu}_f(c)$ compared with when they are assigned to columns with high $\bar{\nu}_f(c)$, we carry out a small simulation study. We consider Bayesian D-optimal and $E(s^2)$-optimal designs of four different sizes from Jones et al. (2008) and Nguyen (1996) and different numbers of active factors. Two different scenarios are considered for each design;

- Scenario 1: The c factors with lowest $\bar{\nu}_f(c)$ are active
- Scenario 2: The c factors with the highest $\bar{\nu}_f(c)$ are active.

Table 3.1: $\bar{\nu}_f(6)$ for individual columns in the $E(s^2)$-optimal design for 30 factors in 18 runs

Column	$\bar{\nu}_f$	Column	$\bar{\nu}_f$
1	1.192	16	1.274
2	1.169	17	1.221
3	1.272	18	1.193
4	1.218	19	1.272
5	1.194	20	1.239
6	1.225	21	1.276
7	1.220	22	1.245
8	1.219	23	1.247
9	1.214	24	1.189
10	1.163	25	1.169
11	1.240	26	1.217
12	1.165	27	1.185
13	1.221	28	1.220
14	1.187	29	1.216
15	1.190	30	1.189

We used $c = n/3$ for all designs except those for 24 factors in 12 runs. This is because, for the design with 24 factors, there were some subsets of four factors for which the VIFs could not be estimated. The simulation operated as follows:

1. Coefficients for *active* factors were simulated from a $N(4, 0.2)$ distribution with their sign chosen randomly.

2. Coefficients for *inactive* factors were simulated from a $N(0, 0.2)$ distribution.

3. Errors, ε, were simulated from a $N(0, 1)$ distribution.

4. Responses, $\mathbf{Y}$ were generated according to the model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, where $\mathbf{X}$ is the design matrix and $\boldsymbol{\beta} = \beta_1, \ldots, \beta_m$ is the vector of coefficients.

5. The data were analysed using the Gauss-Dantzig selector (Candes and Tao, 2007) and the process repeated 2000 times.

Simulating active factors from a $N(4, 0.2)$ distribution means that their coefficients should be comfortably distinguishable from noise (signal to noise ratio = 4). The Gauss-Dantzig selector was shown by Phoa et al. (2009) and Marley and Woods

Table 3.2: Comparing performance of designs when the c factors with lowest $\bar{\nu}_f(c)$ are active (Scenario 1) and c factors with highest $\bar{\nu}_f(c)$ are active (Scenario 2). Power_1 and Power_2 are the proportion of active factors correctly identified under Scenarios 1 and 2. Similarly for Type I error rate_1 and Type I error rate_2.

Design criterion	Runs	Factors	c	$\min_f \bar{\nu}_f(c)$	$\max_f \bar{\nu}_f(c)$	Power_1	Type I error rate_1	Power_2	Type I error rate_2
Bayesian D-opt.	12	16	4	1.095	1.314	0.82	0.07	0.61	0.07
$E(s^2)$-opt.	12	16	4	1.092	1.202	1.00	0.02	0.73	0.09
Bayesian D-opt.	12	18	4	1.141	1.261	0.89	0.06	0.76	0.08
$E(s^2)$-opt.	12	18	4	1.141	1.264	0.85	0.08	0.78	0.09
Bayesian D-opt.	12	24	3	1.111	1.281	0.81	0.07	0.57	0.07
$E(s^2)$-opt.	12	24	3	1.110	1.173	0.99	0.03	0.89	0.05
Bayesian D-opt.	18	30	6	1.157	1.288	0.98	0.04	0.86	0.08
$E(s^2)$-opt.	18	30	6	1.163	1.276	0.93	0.05	0.78	0.08

(2010) to be a promising analysis method for SSDs and hence we use it for the analysis of data from the simulation study, using the tuning parameters detailed in Marley and Woods (2010).

The results are summarised in Table 3.2. Under Scenario 2, the proportion of active factors that we correctly identify (Power_2) is always lower than that under Scenario 1 (Power_1). Also, Type I error rate_2 is always at least as big as Type I error rate_1. Both these points indicate worse performance when factors with higher $\bar{\nu}_f(c)$ are active. For instance, consider the $E(s^2)$-optimal design for 30 factors in 18 runs. We see that Power_2 is 0.78 for this design, which compares rather poorly to a value of 0.93 for Power_1 for the same design. Similarly, the Type I error rate is much higher for Scenario 2 (0.08) than for Scenario 1 (0.04). For the Bayesian D-optimal design for 24 factors the difference in power between the two scenarios is even more dramatic (0.81 for Scenario 1 compared to 0.57 for Scenario 2). These trends are apparent across all the designs considered. We conclude that using prior information to assign factors to columns of the design matrix using $\bar{\nu}_f(c)$ as a criterion may have considerable impact on the success of the screening experiment.

3.3 Combining $\nu_k(\mathcal{S})$ and the A-criterion

Although the application of Criterion 1 will result in a design with good projection properties, in general the designs produced will have sub-optimal accuracy in parameter estimation. In particular, for very unbalanced designs, we can achieve excellent

projection properties at the price of high variances for parameter estimates. Here we describe how to combine $\bar{\nu}(c)$ with another criterion in order to achieve better quality estimates of the parameters.

In Section 3.1.2 it was shown that for the non-supersaturated case

$$\sum_{k=1}^{m} \nu_k = n \sum_{k=1}^{m} \lambda_k^{-1} .$$

This can easily be extended to the supersaturated case. For a given subset, $\mathcal{S}$, of c columns we have

$$\sum_{k=1}^{c} \nu_k(\mathcal{S}) = n \sum_{k=1}^{c} \lambda_k^{-1}(\mathcal{S}) ,$$

where the $\lambda_k(\mathcal{S})$ are the eigenvalues of $\tilde{\boldsymbol{X}}'_{\mathcal{S}}\tilde{\boldsymbol{X}}_{\mathcal{S}}$, where $\tilde{\boldsymbol{X}}_{\mathcal{S}}$ is the standardised design sub-matrix for the columns corresponding to the columns in $\mathcal{S}$.

Now, notice that for two-level balanced designs, $\tilde{\boldsymbol{X}} = \mathbf{X}$, since the column means of $\mathbf{X}$ are all 0 and standard deviations are all 1. Hence,

Result 3: For two-level balanced designs, for each $\mathcal{S}$, $\sum_{k=1}^{c} \nu_k(\mathcal{S})$ is equivalent to the A-optimality objective function on $\mathcal{S}$:

$$\phi_A = \sum_{k=1}^{c} \lambda_k^{-1}(\mathcal{S}) . \tag{3.3}$$

The proof follows directly from Result 2. As a consequence, for balanced two-level designs, Criterion 1 is equivalent to averaging standard A-optimality across different models. This relationship is not true for unbalanced designs. Note that Wu (1993) used a criterion based on averaging A-optimality across different models.

Since $\bar{\nu}(c)$ and the A-criterion are equivalent for two-level balanced designs, we combine these two criteria to form a compound criterion to find potentially unbalanced designs in which factors are not restricted to only two levels. To promote a degree of balance in the designs (and hence low confounding with the overall mean), we modify (3.3) so that every sub-matrix considered also includes a column of 1s, or intercept column. The modification gives the following:

$$A(c) = \frac{1}{(c+1)m'} \sum_{l=1}^{m'} tr(([\mathbf{1}|\mathbf{X}_{\mathcal{S}_l}]'[\mathbf{1}|\mathbf{X}_{\mathcal{S}_l}])^{-1}), \tag{3.4}$$

where $\mathbf{X}_{\mathcal{S}_l}$ is the design sub-matrix for the columns corresponding to the numbers in $\mathcal{S}_l$. This means that imbalance in the columns of the design will increase the value of the criterion.

A possible compound criterion is the following:

$$\text{Criterion 3:} \qquad minimise \quad \bar{\nu}_A(c) = w_A log(A(c)) + w_V log(\bar{\nu}(c)),$$

where w_V and w_A are weights with $w_V + w_A = 1$. Increasing w_V places more weight on $\bar{\nu}(c)$ and indicates the experimenter is more willing to accept higher variances for parameter estimators in return for less multifactor dependency. We note that reducing w_V will tend to result in more balance in the designs. Marley and Woods (2010) showed that slightly unbalanced SSDs can perform very well and hence we do not consider perfect balance to be a necessity. However, it is important that the designs are not so unbalanced as to result in large confounding with the overall mean.

We consider an extension of Criterion 3 which allows us to consider subsets of factors of differing sizes. For instance, suppose the experimenter thinks that either two, three or four factors are likely to be active. Then he may wish to base his design on a weighted combination of $\bar{\nu}(2)$, $\bar{\nu}(3)$ and $\bar{\nu}(4)$, as well as $A(2)$, $A(3)$ and $A(4)$. Hence we consider different weights, w_c, on different values of c, with $\sum_{c=2}^{c_{max}} w_c = 1$, where c_{max} is the maximum number of factors the experimenter believes could be active. The weights reflect the prior beliefs of the experimenter of how many factors will be active.

We define a criterion in terms of $\bar{\nu}^{c_{max}}$ and $A^{c_{max}}$:

$$\text{Criterion 4:} \qquad maximise \quad \bar{\nu}_A^{c_{max}} = w_A log(A^{c_{max}}) - w_V log(\bar{\nu}^{c_{max}}),$$

where

$$\bar{\nu}^{c_{max}} = \sum_{c=2}^{c_{max}} w_c \bar{\nu}(c)\,,$$

$$A^{c_{max}} = \sum_{c=2}^{c_{max}} w_c A^*(c)/A(c)\,,$$

and

$$A^*(c) = tr(n\mathbf{I}_{c+1})^{-1}\,. \tag{3.5}$$

Here $\mathbf{I}_i$ is the identity matrix with i rows.

As the variance inflation factors represent a *proportional* change, we use simply a weighted average of $\bar{\nu}(c)$ in Criterion 4. However, since the variances represented by $A(c)$ are *absolute* values, we consider $A(c)$-efficiency, which is also a proportional value. The baseline we use for $A(c)$-efficiency is $A^*(c)$, shown in (3.5). This is the trace of the (typically unachievable) information matrix we would have if there were no dependencies between columns. Hence our $A(c)$-efficiency is given by $A^*(c)/A(c)$.

Criterion 4 is a product criterion, maximising the product of the efficiencies of the two different parts of the criterion, using the specified weights, see Läuter (1974). The signs for the A and the $\bar{\nu}$ part are different since we wish to minimise $\bar{\nu}^{c_{max}}$ but maximise the efficiency, $A^{c_{max}}$. This is in contrast to Criterion 3, where we also wished to minimise the raw value of $A(c)$. How to choose appropriate weights is considered in more detail in Section 3.5. Criterion 4 is used to generate new SSDs in Sections 3.4 and 3.5.

3.4 Generating supersaturated designs with independent combinations of factor levels

In this section, we generate some new mid-size two-level and three-level SSDs using Criterion 4. This will lead into design generation for a more interesting case in Section 3.5 where factor levels cannot be set independently. The coordinate exchange algorithm (Meyer and Nachtsheim, 1995) is used to generate all designs discussed in this section.

Table 3.3: Comparison of designs for 16 factors and 12 runs under $\bar{\nu}(4)$, $A^*(4)/A(4)$, $E(s^2)$ and ϕ_D.

Design	$\bar{\nu}(4)$	$A^*(4)/A(4)$	$E(s^2)$	$\phi_D^{1/(m+1)}$
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.25$	1.1376	0.8864	4.93	4.54
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.5$	1.1376	0.8864	4.93	4.54
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.75$	1.1376	0.8864	4.93	4.54
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.9$	1.1376	0.8864	4.93	4.54
$E(s^2)$-opt.	1.1574	0.8881	5.2	4.53
Bayesian D-opt.	1.1462	0.8748	4.8	4.55

Table 3.4: Comparison of designs for 18 factors and 12 runs under $\bar{\nu}(4)$, $A^*(4)/A(4)$, $E(s^2)$ and ϕ_D.

Design	$\bar{\nu}(4)$	$A^*(4)/A(4)$	$E(s^2)$	$\phi_D^{1/(m+1)}$
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.25$	1.1744	0.8686	5.86	3.50
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.5$	1.1646	0.8661	5.44	3.51
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.75$	1.1646	0.8661	5.44	3.51
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.9$	1.1646	0.8661	5.44	3.51
$E(s^2)$-opt.	1.1817	0.8731	5.96	3.51
Bayesian D-opt.	1.1819	0.8729	5.96	3.51

3.4.1 Two-level designs using Criterion 4

Designs were created for 16, 18 and 24 factors in 12 runs using Criterion 4 with $w_4 = 1$ (all weight on four factors) using multiple random starts of the coordinate exchange algorithm. Four different weights w_V were used: $w_V = 0.25$, 0.5, 0.75 and 0.9. Tables 3.3, 3.4 and 3.5 show how the new designs for 16, 18 and 24 factors compare with those of the same size generated by Jones et al. (2008) using Bayesian D-optimality and Nguyen (1996) using $E(s^2)$-optimality. Nguyen's designs meet the $E(s^2)$ lower bound provided by Ryan and Bulutoglu (2007). Notice that in some cases the design of Jones et al. (2008) performs better than that of Nguyen (1996) under $E(s^2)$ despite being generated using a different criterion. This is due to Nguyen's designs being constrained to be balanced. The value of $\tau^2 = 5$ was used in the Bayesian D-optimality criterion in order to match with Jones et al. (2008).

We see from Tables 3.3 - 3.5 that all the designs generated under Criterion 4 outperform both the Bayesian D-optimal and $E(s^2)$-optimal designs for all w_V, when

Table 3.5: Comparison of designs for 24 factors and 12 runs under $\bar{\nu}(4)$, $A^*(4)/A(4)$, $E(s^2)$ and ϕ_D. A * indicates that one or more sub-matrices of four columns had rank of less than four.

Design	$\bar{\nu}(4)$	$A^*(4)/A(4)$	$E(s^2)$	$\phi_D^{1/(m+1)}$
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.25$	1.2441	0.8366	8.00	2.00
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.5$	1.2413	0.8382	7.94	2.00
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.75$	1.2396	0.8345	7.81	2.00
$\bar{\nu}_A^4$, $w_4 = 1$, $w_V = 0.9$	1.2396	0.8345	7.65	2.00
$E(s^2)$-opt.	*	*	7.83	2.01
Bayesian D-opt.	*	*	7.83	2.01

comparing using $\bar{\nu}(4)$, indicating that we have produced designs with lower multi-factor dependencies. In the 16 factor case we see considerable improvement in $\bar{\nu}(4)$ over the corresponding $E(s^2)$-optimal design (1.1376 compared to 1.1574). At the same time, they perform very similarly to each other under ϕ_D (shown in (3.2)) and have good values of $E(s^2)$, particularly when there are 18 factors. The designs for 16 and 18 factors seem particularly insensitive to the choice of w_V, often producing the same design properties for different w_V.

Notice that there are some combinations of four factors for which the design submatrix has rank less than four in the 24 factor Bayesian D-optimal and $E(s^2)$-optimal designs. This means that model parameters are not estimable for some four factor projections. In contrast to this, our new designs for 24 factors ensure estimability for all four factor projections. Table 3.5 shows that we lose very little under Bayesian D-optimality in order to achieve this and in fact we can also improve under $E(s^2)$-optimality. More generally, Criterion 4 ensures that all models including up to c_{max} factors are estimable. This is a considerable advantage over the $E(s^2)$-optimal and Bayesian D-optimal designs and links to the model-robust supersaturated designs explored by Jones et al. (2009). For fixed n and m they considered the maximum number of factors, g, such that all models including g factors were estimable and present designs achieving this estimability property. They also present a subspace angle criterion for evaluating their designs. They use this as a measure of how well two models can be distinguished from each other in their designs.

Another point worthy of note is that as w_V increases (i.e. as we place less weight on

Table 3.6: Design for 18 factors and 12 runs generated using Criterion 4 with $w_4 = 1$ and $w_V = 0.5$

	Factor																	
Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1	-1	-1	1	-1	-1	1	-1	-1	1	1	1	1	1	-1	-1	-1	-1
2	-1	1	1	1	1	1	-1	1	1	-1	1	1	1	1	-1	1	-1	-1
3	1	1	1	1	-1	-1	1	1	1	1	1	-1	-1	1	-1	1	1	1
4	-1	-1	-1	1	-1	1	-1	1	-1	1	1	-1	1	-1	1	1	-1	1
5	1	-1	-1	-1	1	-1	-1	1	-1	-1	-1	-1	-1	1	-1	1	-1	-1
6	1	-1	1	1	1	-1	-1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
7	-1	-1	-1	1	-1	1	1	1	1	-1	-1	1	-1	-1	-1	-1	1	-1
8	-1	1	1	1	1	1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1	-1
9	1	1	-1	-1	-1	1	-1	-1	1	1	-1	1	1	1	1	1	1	-1
10	-1	1	-1	-1	1	-1	1	1	-1	-1	1	1	1	1	1	-1	1	1
11	1	1	1	-1	-1	1	-1	-1	-1	-1	1	1	-1	-1	-1	-1	-1	1
12	-1	-1	1	-1	1	-1	1	-1	1	1	-1	1	1	-1	-1	1	-1	1

the A-optimality part of the criterion) the designs may contain more columns which are unbalanced. For instance, with $w_V = 0.25$, the design for 18 factors contains four unbalanced columns. This increases to 8 unbalanced columns for $w_V = 0.5$. The design for 18 factors generated with $w_v = 0.5$ is given in Table 3.6. The $E(s^2)$-optimal designs tend to have good values of $A^*(4)/A(4)$ since they are balanced.

3.4.2 Two-level designs using $\tilde{\nu}(c)$

If we wished to minimise the impact of a worst case scenario occurring, then we could incorporate maximum VIFs into the design construction criterion.

$$\text{Criterion 5:} \qquad minimise \quad \tilde{\nu}_A^{c_{max}} = w_A log(A^{c_{max}}) - w_V log(\tilde{\nu}^{c_{max}}) \,,$$

where

$$\tilde{\nu}^{c_{max}} = \sum_{c=1}^{c_{max}} w_c \tilde{\nu}(c) \,.$$

We generated designs for 16, 18 and 24 factors in 12 runs using Criterion 5 with $w_V = 0.25$, 0.5, 0.75 and 0.9, and $w_3 = 1$. These designs all have a maximum VIF of 1.5, which matches that of the corresponding $E(s^2)$-optimal designs and either

matches or beats those of the Bayesian D-optimal designs (1.89, 1.5 and 3 for 16, 18 and 24 factors respectively).

3.4.3 Three-level designs

In some experiments, particularly when categorical variables are present, an experimenter may wish to consider using a multi-level or a mixed-level SSD. In such cases, it is still desirable to consider multi-factor dependencies and hence we now use Criterion 4 to generate some new three-level SSDs for 16 factors in 9 runs. We set $w_3 = 1$ and consider $w_V = 0.1$, 0.25, 0.5 and 0.75. As a comparison we inspect a design of the same size from Xu and Wu (2005) which is optimal under the Generalised Minimum Aberration criterion, and also equivalently the $ave\chi^2$ criterion:

$$ave\chi^2 = \sum_{1 \le i < j \le m} \chi^2(c_i, c_j)/[m(m-1)/2]\,,$$

where

$$\chi^2(c_i, c_j) = \sum_{a=0}^{s_i-1} \sum_{b=0}^{s_j-1} [n_{ab}^{ij} - n/s_i s_j]^2/(n/(s_i s_j))\,.$$

Columns i and j are denoted by c_i and c_j and have number of levels s_i and s_j. The number of times that pair (a, b) appears in columns c_i and c_j is given by n_{ab}^{ij}. Notice that this criterion only considers the average dependency between *pairs* of columns.

Table 3.7 indicates that our designs perform better than Xu and Wu's under $\bar{\nu}(3)$ even for low w_V. As expected, Xu and Wu's design performs better under $ave\chi^2$. It is interesting to compare columns 1 and 5 from Table 3.7, which evaluate the designs under $\bar{\nu}(2)$ and $ave\chi^2$. Both of these criteria in some way evaluate the dependencies between pairs of columns in the design matrix and yet they give different conclusions as to which design is best. When such a disagreement occurs, it is generally best to use the $\bar{\nu}(2)$ design since this criterion has the greater practical interpretability. Our new design with $w_V = 0.1$ is given in Table 3.8.

Table 3.7: Comparison of three-level designs for 16 factors and 9 runs.

Design	$\bar{\nu}(2)$	$\bar{\nu}(3)$	$A^*(2)/A(2)$	$A^*(3)/A(3)$	$ave\chi^2$
$\bar{\nu}_A^3$, $w_3 = 1$, $w_V = 0.1$	1.1355	1.3401	0.9206	0.8083	3.80
$\bar{\nu}_A^3$, $w_3 = 1$, $w_V = 0.25$	1.1250	1.3061	0.9191	0.8069	3.93
$\bar{\nu}_A^3$, $w_3 = 1$, $w_V = 0.5$	1.1250	1.3061	0.9191	0.8069	3.93
$\bar{\nu}_A^3$, $w_3 = 1$, $w_V = 0.75$	1.1056	1.2497	0.9155	0.8029	4.23
Xu and Wu	1.1580	1.3840	0.9172	0.8004	3.60

Table 3.8: Three-level design for 16 factors and 9 runs generated using criterion $\bar{\nu}_A^3$ with $w_V = 0.1$

	Factor															
Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1	2	1	2	1	2	1	0	0	1	0	0	2	0	0	0
2	2	1	2	0	2	1	0	0	0	1	2	2	1	2	1	0
3	0	1	1	2	0	2	2	1	1	0	1	1	1	0	1	0
4	0	0	0	1	2	0	2	2	0	0	0	2	1	2	0	2
5	2	1	1	1	0	0	0	1	2	2	1	0	2	1	0	2
6	1	0	2	0	0	1	2	0	2	2	0	1	0	0	2	2
7	2	0	2	1	1	2	1	2	1	0	1	0	0	2	2	1
8	0	2	0	0	1	0	0	1	1	2	2	2	2	0	2	1
9	1	2	0	2	2	1	1	2	2	1	2	1	0	1	1	1

Table 3.9: Four solvents with 8 chemical properties from Ballistreri et al. (2002)

	Property							
Solvent	1	2	3	4	5	6	7	8
1	0.66	-0.47	0.40	-0.12	-0.97	1.00	-0.50	-0.96
2	0.69	0.40	1.00	0.67	-0.19	0.60	-0.12	-1.00
3	0.50	0.29	-0.34	0.15	-0.30	0.58	-0.20	-0.95
4	-0.59	-0.74	-0.44	-0.18	-1.00	0.52	-0.73	-0.78

3.5 ν_A-optimal supersaturated designs where factor levels cannot be set independently

We now consider a situation which often occurs when experiments involve chemical compounds. There is a candidate list of compounds, all having different chemical properties, for example melting point or boiling point. These properties are the factors to be varied in an experiment through choosing one compound for each run of an experiment. In this section, Criterion 4 is used to construct SSDs for two such examples from chemistry.

3.5.1 Example 1

We design supersaturated experiments for a list of solvents from Ballistreri et al. (2002). They document over 100 solvents and detail several descriptors and principal properties for each. After removing solvents with missing values, we were left with a candidate list of 81 solvents and 9 properties. However, properties 8 and 9 (lipophilicity and water solubility) were highly correlated and hence water solubility was not considered. Table 3.9 shows the remaining 8 properties of four of the solvents. Notice that all the properties have been scaled to lie between -1 and 1. Such an experiment differs from those discussed in Section 3.4 since the particular solvent used for a given run determines the levels of all the factors for that run.

We use Criterion 4 to design an experiment of 6 runs for the remaining 8 properties. We take $c_{max} = 3$ and apply 3 sets of weights on different numbers of active factors; $(w_2, w_3) = (0.25, 0.75)$, $(0.5, 0.5)$ and $(0.75, 0.25)$. For each of these weights we use $w_V = 0, 0.1, \ldots, 0.9, 1$. All designs were constructed using an exchange algorithm

Table 3.10: Design for the solvent candidate list for $(w_2, w_3) = (0.5, 0.5)$ and $w_V = 0$

	Factor							
Run	1	2	3	4	5	6	7	8
1	0.66	-0.47	0.40	-0.12	-0.97	1.00	-0.50	-0.96
2	0.26	0.22	-0.95	-0.30	0.98	-0.68	1.00	0.44
3	0.69	0.40	1.00	0.67	-0.19	0.60	-0.12	-1.00
4	-1.00	-0.96	-1.00	-1.00	-0.80	-1.00	-1.00	0.49
5	0.40	0.05	-0.34	0.85	-0.25	-0.25	-0.48	-0.78
6	1.00	0.77	-0.97	-0.42	0.69	-0.74	-0.25	0.74

Table 3.11: Design for the solvent candidate list for $(w_2, w_3) = (0.5, 0.5)$ and $w_V = 0.4$

	Factor							
Run	1	2	3	4	5	6	7	8
1	0.69	0.40	1.00	0.67	-0.19	0.60	-0.12	-1.00
2	-0.59	-0.74	-0.44	-0.18	-1.00	0.52	-0.73	-0.78
3	0.49	0.24	-0.57	1.00	0.36	-0.35	-0.36	-0.07
4	0.26	0.22	-0.95	-0.30	0.98	-0.68	1.00	0.44
5	0.11	0.28	-0.99	-1.00	0.04	-0.98	-0.55	1.00
6	0.81	-0.46	-0.99	-0.78	-0.36	-0.70	-0.32	-0.62

(see for instance Cook and Nachtsheim, 1980) and were the best out of 100 random starts.

Tables 3.10, 3.11 and 3.12 show the designs for $(w_2, w_3) = (0.5, 0.5)$ with $w_V = 0$, $w_V = 0.4$ and $w_V = 1$. The design with $w_V = 0$ corresponds to generating only under A^3. Similarly, $w_V = 1$ corresponds to generating only under $\bar{\nu}^3$. Table 3.13 shows $\bar{\nu}(2)$, $\bar{\nu}(3)$, $A^*(2)/A(2)$ and $A^*(3)/A(3)$ for the designs with $w_V = 0, 0.1, \ldots, 0.9, 1$.

As expected, Table 3.13 shows that the $\bar{\nu}$ values of the designs improve (decrease) as w_V increases (that is as we place more weight on $\bar{\nu}^3$). Similarly, $A^*(c)/A(c)$, $c = 2, 3$ deteriorates (decreases) as w_V increases. It can be seen from Table 3.10 that having more weight on the A-optimality part of the criterion results in a design with a much wider spread of the factor levels. Notice that all the factors have at least one value close to 1 and one close to -1. Contrast this with Factor 3 in Table 3.12 which has no value greater than -0.69. However, the wider spread of factor levels in Table 3.10 comes at the expense of much larger linear dependencies amongst the factors,

Table 3.12: Design for the solvent candidate list for $(w_2, w_3) = (0.5, 0.5)$ and $w_V = 1$

	Factor							
Run	1	2	3	4	5	6	7	8
1	-0.58	-0.80	-0.85	-0.09	-0.40	-0.47	-0.09	0.00
2	0.07	0.07	-0.85	0.33	-0.43	-0.56	-0.70	0.36
3	-0.34	-0.17	-0.78	-0.15	-0.45	0.17	-0.69	-0.07
4	-0.45	-0.63	-0.69	0.37	-0.66	-0.35	-0.70	-0.45
5	0.54	-0.45	-0.93	-0.15	-0.48	-0.37	-0.70	-0.27
6	0.13	-0.35	-0.80	0.18	0.24	-0.41	-0.41	-0.34

Table 3.13: Comparison of designs for the solvent candidate list for $(w_2, w_3) = (0.5, 0.5)$ and $w_V = 0, 0.1, \ldots, 0.9, 1$

w_V	$\bar{\nu}(2)$	$\bar{\nu}(3)$	$A^*(2)/A(2)$	$A^*(3)/A(3)$
0	1.86	3.37	0.32	0.18
0.1	1.42	2.27	0.30	0.18
0.2	1.42	2.27	0.30	0.18
0.3	1.42	2.27	0.30	0.18
0.4	1.42	2.27	0.30	0.18
0.5	1.42	2.27	0.30	0.18
0.6	1.38	1.99	0.26	0.17
0.7	1.31	1.87	0.24	0.16
0.8	1.29	1.73	0.20	0.14
0.9	1.17	1.49	0.10	0.07
1	1.14	1.43	0.02	0.02

as shown by the higher $\bar{\nu}(c)$. In Table 3.11 we see a slightly wider spread of factor levels for $w_V = 0.4$ than when $w_V = 1$. Also the design provides a good compromise between $\bar{\nu}(c)$ and $A(c)$. For instance, Table 3.13 shows $\bar{\nu}(2) = 1.42$ for $w_V = 0.4$ compared to 1.86 for $w_V = 0$ and 1.14 when $w_V = 1$.

Table 3.13 also illustrates that small changes in w_V may not change the resulting design properties. In fact, the designs for $w_V = 0.1, 0.2, \ldots, 0.5$ are all the same.

One task facing an experimenter is to choose which value of w_V to use. We recommend generating a design for each of the 11 values of w_V used above and constructing efficiency plots for a given (w_2, w_3) based on the best possible design under $\bar{\nu}^{c_{max}}$, and the best possible design under $A^{c_{max}}$ (that is with $w_V = 1$ and $w_V = 0$). Let ξ_1 be the $\bar{\nu}^{c_{max}}$-optimal design and ξ_0 be the $A^{c_{max}}$-optimal design. Then, if ξ is any design, the $\bar{\nu}^{c_{max}}$-efficiency is defined as

$$\bar{\nu}^{c_{max}}(\xi_1)/\bar{\nu}^{c_{max}}(\xi)\,,$$

where $\bar{\nu}^{c_{max}}(\xi)$ is the value of $\bar{\nu}^{c_{max}}$ for design ξ. Similarly, the $A^{c_{max}}$-efficiency is defined as

$$A^{c_{max}}(\xi)/A^{c_{max}}(\xi_0)\,.$$

Efficiency plots for $(w_2, w_3) = (0.5, 0.5)$, $(0.25, 0.75)$ and $(0.75, 0.25)$ are shown in Figures 3.1-3.3. These graphs illustrate how $\bar{\nu}^{c_{max}}$ and $A^{c_{max}}$ vary relative to their best possible values as w_V changes. Obviously, as w_V increases, $\bar{\nu}^{c_{max}}$-efficiency increases and $A^{c_{max}}$-efficiency decreases. The plots help to illustrate the different trade-offs made between $\bar{\nu}(c)$ and the A-optimality. Consider, for instance, Figure 3.3 which shows the efficiency plot for $(w_2, w_3) = (0.75, 0.25)$. When $w_V = 0$ we naturally see a very poor $\bar{\nu}^{c_{max}}$-efficiency (0.54). However, increasing w_V to 0.1 results in a large increase in $\bar{\nu}^{c_{max}}$-efficiency (0.74) with only a small reduction in $A^{c_{max}}$-efficiency (from 1 to 0.97). This may be a suitable choice of w_V since the average of the two efficiencies is at it's highest, but the experimenter should consider his or her own objectives when making the choice.

Figure 3.1: $\bar{\nu}^{c_{max}}$- (dashed line) and $A^{c_{max}}$- (dotted line) efficiencies for designs from the solvent candidate list with $(w_2, w_3) = (0.5, 0.5)$. Solid line is the average of the two efficiencies.

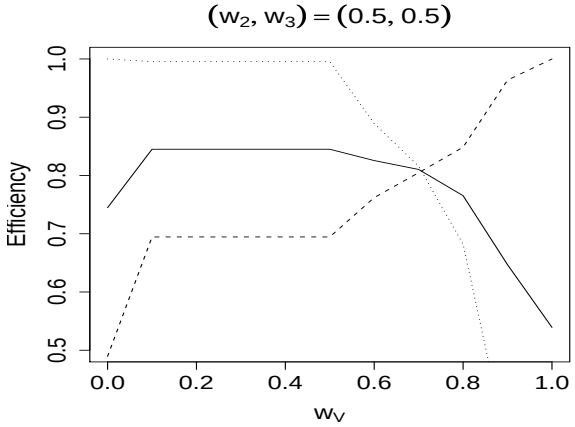
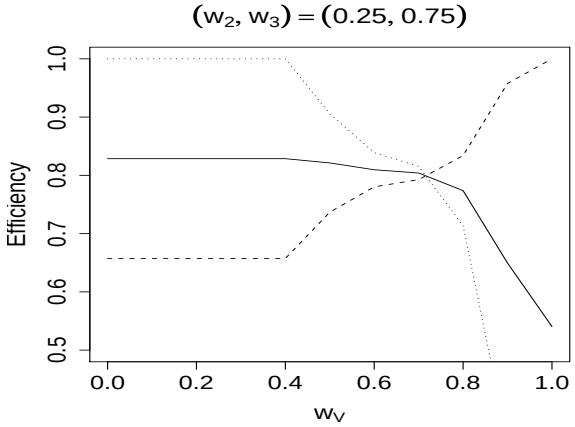


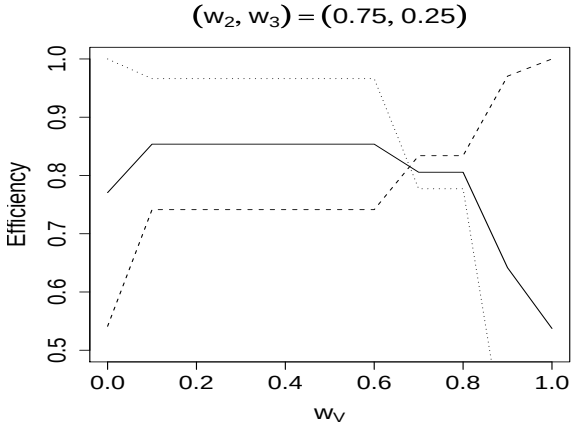
Figure 3.2: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the solvent candidate list with $(w_2, w_3) = (0.25, 0.75)$. Solid line is the average of the two efficiencies.



Notice in Figures 3.1-3.3 how $A^{c_{max}}$-efficiency drops sharply when $w_V > 0.8$ and thus using a design with w_V in this range for this candidate list is not recommended.

Another issue for the experimenter is to choose values of $w_2, w_3, \ldots, w_{c_{max}}$. In all cases, the weights and the choice of c_{max} should reflect the assumption of effect sparsity (only a small proportion of the factors are active). Unless some prior information is available that certain factors are active, the choice should place high weights on low values of c. The choice of equal weights up to a (relatively low) c_{max} will provide a design which is more robust to variation in the true number of active factors. Hence $(w_2, w_3) = (0.5, 0.5)$ or $(0.75, 0.25)$ are reasonable choices here. For this candidate list, the design which maximises the average efficiency is the

Figure 3.3: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the solvent candidate list with $(w_2, w_3) = (0.75, 0.25)$. Solid line is the average of the two efficiencies.



same across all three sets of weights (w_2, w_3) considered. This indicates insensitivity to reasonable choice of (w_2, w_3), although this need not be the case for different candidate sets.

As a comparison, a Bayesian D-optimal design for the same candidate list was generated. This has $\bar{\nu}(2) = 1.83$, $\bar{\nu}(3) = 4.80$, $A^*(2)/A(2) = 0.29$ and $A^*(3)/A(3) = 0.08$. Comparing with the figures in Table 3.13 we see that our new designs are clearly better, particularly if there are three active factors.

We also demonstrate the advantages of Criterion 4 over the $E(s^2)$ criterion. Further to only incorporating pairwise relationships between the columns of the design, $E(s^2)$ has a particular shortcoming when designing experiments where the factor levels are not just ± 1. We illustrate this through an example.

We pursue the 8-factor, 6-run set-up of the solvent example but now suppose that there is a solvent (Solvent Z) with the following factor levels:

Property	1	2	3	4	5	6	7	8
Solvent Z	0.00	0.01	0.02	0.00	0.00	0.01	0.01	0.02

Now suppose further that we construct a design with Solvent Z chosen for each of the six runs. This design has $E(s^2) = 0.00000055$. This compares to a value of 3.05 for the Bayesian D-optimal design and 1.31 for the ν_A-optimal design with $w_V = 4$ and $(w_2, w_3) = (0.5, 0.5)$. Thus, the design with Solvent Z has a far better value of

$E(s^2)$ than the two other designs. However, it is clearly not a good design to use, primarily because all runs are the same, so we cannot estimate the effects of any of the factors. This illustrates that $E(s^2)$ is not a sensible criterion to use for this type of experiment. As shown by the example, a good value of $E(s^2)$ can be obtained by designing an experiment using only entries from the candidate list which have values of the factor levels relatively close to zero. This can result in designs with poor accuracy in parameter estimation and the possibility of not being able to fit some models involving only a very small number of factors.

3.5.2 Example 2

We now consider a list of 270 compounds provided by the Lubrizol Corporation. Lubrizol measured 10 properties for each compound and desired to know which (if any) of the properties had a substantial effect on a response of interest. We use Criterion 4 to generate some 8-run designs. We use $c_{max} = 4$ and consider 4 sets of weights on different numbers of active factors; $(w_2, w_3, w_4) = (1/3, 1/3, 1/3)$, $(0.5, 0.3, 0.2)$, $(0.8, 0.1, 0.1)$ and $(0.1, 0.1, 0.8)$. Again, for each of these weights we consider $w_V = 0, 0.1, \ldots, 0.9, 1$. The four efficiency graphs corresponding to the four different sets of weights are shown in Figures 3.4-3.7. In these plots, we see similar trends as for Figures 3.1-3.3. For this candidate list, the design for which the average efficiency is maximised depends on the weights (w_2, w_3, w_4).

Tables 3.14 and 3.15 show $\bar{\nu}(2)$, $\bar{\nu}(3)$, $\bar{\nu}(4)$, $A^*(2)/A(2)$, $A^*(3)/A(3)$ and $A^*(4)/A(4)$ for $(w_2, w_3, w_4) = (1/3, 1/3, 1/3)$ and $(0.5, 0.3, 0.2)$ with $w_V \leq 0.8$. It can be seen that the properties of the two sets of designs are very similar, illustrating that small changes in the weights (w_2, w_3, w_4) tend not to produce large changes in the design.

As with the solvent candidate list in Example 1, we generate a Bayesian D-optimal design for the Lubrizol compound example. In this case, the same design as for $w_V = 0$ for all four (w_2, w_3, w_4) was produced.

Figure 3.4: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the Lubrizol compound candidate list with $(w_2, w_3, w_4) = (1/3, 1/3, 1/3)$. Solid line is the average of the two efficiencies.

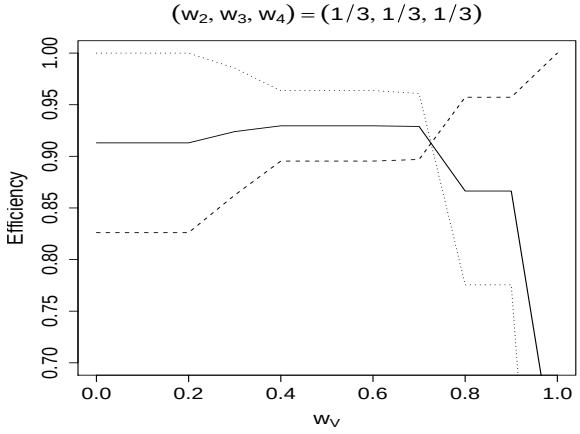


Figure 3.5: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the Lubrizol compound candidate list with $(w_2, w_3, w_4) = (0.5, 0.3, 0.2)$. Solid line is the average of the two efficiencies.

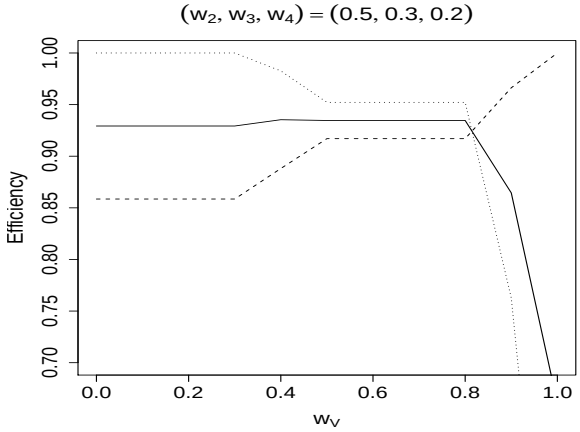


Figure 3.6: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the Lubrizol compound candidate list with $(w_2, w_3, w_4) = (0.8, 0.1, 0.1)$. Solid line is the average of the two efficiencies.

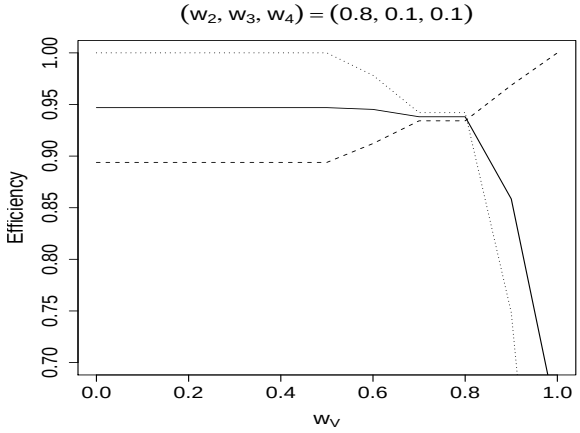


Figure 3.7: $\bar{\nu}^{c_{max}}$ (dashed line) and $A^{c_{max}}$ (dotted line) efficiencies for designs from the Lubrizol compound candidate list with $(w_2, w_3, w_4) = (0.1, 0.1, 0.8)$. Solid line is the average of the two efficiencies.

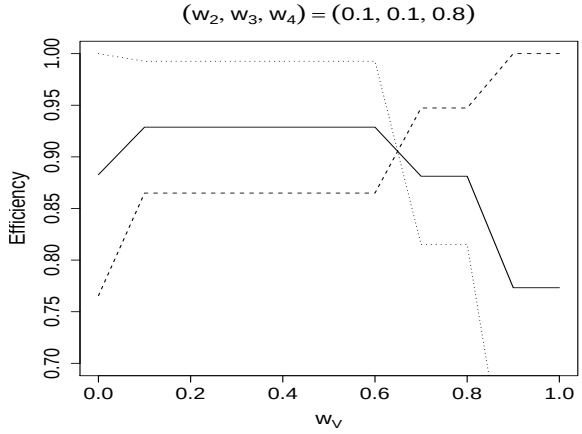


Table 3.14: Comparison of designs for the Lubrizol compound candidate list for $(w_2, w_3, w_4) = (1/3, 1/3, 1/3)$ and $w_V = 0, 0.1, \ldots, 0.7, 0.8$

w_V	$\bar{\nu}(2)$	$\bar{\nu}(3)$	$\bar{\nu}(4)$	$A^*(2)/A(2)$	$A^*(3)/A(3)$	$A^*(4)/A(4)$
0	1.14	1.37	1.78	0.29	0.23	0.17
0.1	1.14	1.37	1.78	0.29	0.23	0.17
0.2	1.14	1.37	1.78	0.29	0.23	0.17
0.3	1.13	1.32	1.66	0.28	0.22	0.17
0.4	1.12	1.29	1.55	0.27	0.22	0.17
0.5	1.12	1.29	1.55	0.27	0.22	0.17
0.6	1.12	1.29	1.55	0.27	0.22	0.17
0.7	1.11	1.28	1.56	0.27	0.22	0.17
0.8	1.09	1.21	1.40	0.21	0.18	0.14

Table 3.15: Comparison of designs for the Lubrizol compound candidate list for $(w_2, w_3, w_4) = (0.5, 0.3, 0.2)$ and $w_V = 0, 0.1, \ldots, 0.7, 0.8$

w_V	$\bar{\nu}(2)$	$\bar{\nu}(3)$	$\bar{\nu}(4)$	$A^*(2)/A(2)$	$A^*(3)/A(3)$	$A^*(4)/A(4)$
0	1.14	1.37	1.78	0.29	0.23	0.17
0.1	1.14	1.37	1.78	0.29	0.23	0.17
0.2	1.14	1.37	1.78	0.29	0.23	0.17
0.3	1.14	1.37	1.78	0.29	0.23	0.17
0.4	1.13	1.32	1.66	0.28	0.22	0.17
0.5	1.11	1.28	1.56	0.27	0.22	0.17
0.6	1.11	1.28	1.56	0.27	0.22	0.17
0.7	1.11	1.28	1.56	0.27	0.22	0.17
0.8	1.11	1.28	1.56	0.27	0.22	0.17

3.6 Discussion

We have shown that variance inflation factors can be a useful tool when considering supersaturated designs. They can easily be used to assess existing competing designs and can also give an indication of which factors should be assigned to which columns when some prior information is available. VIFs can also be incorporated into widely applicable criteria used to generate designs where the factors are at two or more levels, or where their levels cannot be set independently.

In the two-level case, we show that our new designs perform favourably in many cases compared with existing alternatives. By using Criterion 4 and allowing some imbalance in the designs, we can often achieve good VIFs and $E(s^2)$ values.

A considerable advantage of considering VIFs is that we are not restricted to looking only at dependencies between pairs of factors (as we are with $E(s^2)$). This is particularly beneficial when considering mid-size experiments, where there could reasonably be three or four active factors.

We have shown that the weight, w_V, on $\bar{\nu}(c)$ in compound Criterion 4 can be adjusted to the requirements of a particular experiment, in order to achieve more balance, a broader spread of the factors, or less linear dependency between the columns. This makes our criterion more flexible than some existing approaches.

Unless strong prior information that some factors are active is available, we recommend setting $(w_2, w_3, \ldots, w_{c_{max}}) = (1/(c_{max}-1), 1/(c_{max}-1), \ldots, 1/(c_{max}-1))$ as such a design will give more uniform performance across different numbers of true active factors.

The sacrifice required in order to achieve the advantages of the variance inflation factor based criteria is the computational time required to find the designs. Because so many models are being considered, computational restrictions may prohibit the generation of large designs, particularly if we wish to incorporate five or more active factors into the criterion. However, as computer time is generally cheap compared to experimentation, the advantages of the new designs could make this investment of time worthwhile.

Chapter 4

Supersaturated experiments for screening interaction effects with application to robust product design

Interactions between control and noise factors are often utilised in robust product design. Experiments can be designed to find settings of the control factors that dampen the variability in the response due to variability in the noise factors by exploiting control by noise interactions. One problem with such experiments is that, even for a moderate number of control and noise factors, a large number of interactions will be of interest. Traditional methods of planning experiments result in plans with many runs, which can be costly. In such a situation, an alternative is a supersaturated experiment, in which the number of observations is less than the number of factorial effects requiring estimation.

A new criterion for constructing supersaturated designs with both control and noise factors is described. By allowing complete aliasing between effects that are not of interest, the criterion results in designs with only minimal partial aliasing between effects of interest. A flexible algorithmic approach is used to find designs for any number of control and noise factors, and also any run size. The performance of the new designs in relation to competing methods is discussed and some examples are presented to illustrate, in particular, how the new designs have a higher power to detect those effects of interest that have a substantive impact on the response.

4.1 Introduction

In industrial experimentation a key tool for improving quality of products and processes is the exploitation of interactions between so called control factors (denoted C) and noise factors (denoted N). Control factors can be set in the product specification, whereas noise factors cannot. However, it is often possible to mimic the noise factors in an experiment, and hence provide useful information on control by noise ($C \times N$) interactions. Many such experiments have been discussed in the literature, for example Miller et al. (1993) described an experiment in automobile manufacturing. An experiment with five control and three noise factors was conducted to try to find settings of the control factors which resulted in minimal distortion of the drive pinion and gear set under heat treatment. Vine et al. (2008) described an experiment to identify important factors affecting the cold start performance of a new generation engine at Jaguar cars. Reducing performance variability was important and as such, both control and noise factors were involved. A group screening approach was pursued, whereby factors under investigation are partitioned into groups. In each run, all factors within a group are set to the same level and hence factors within the same group are completely confounded with each other.

Robust design was first discussed by Taguchi (1986) who proposed crossing two design matrices (arrays); one for control factors and one for noise factors. However, this approach was criticised because the number of runs required was often prohibitively large. Welch et al. (1990) proposed using a combined array, incorporating both control and noise factors. This idea was then further explored by Shoemaker et al. (1991), who illustrated how a combined array can result in smaller experiments. More recently, Wu and Zhu (2003) and Zhu et al. (2007) have proposed aberration-type criteria to choose the best combined array. One of the drawbacks is that many of these designs have effects of interest which are completely aliased with other effects. Loeppky et al. (2006) also proposed an aberration-type criterion for non-regular designs. These have main effects and two-factor interactions which are partially aliased. Kang and Joseph (2009) proposed a Bayesian criterion for selecting the optimal combined array. This criterion incorporated the concept of effect hierarchy in addition to reflecting the differing importance of certain effects. The

criterion focussed on efficient estimation of the variance and as such places much emphasis on noise main effects and control by noise interactions. However, the authors acknowledge that the criterion could be altered to allow better estimation of the mean of the process. The designs could have any number of runs and may also be non-regular. Lewis and Dean (2001) instead used two-stage group screening to provide information on important interactions.

Supersaturated experiments traditionally have more factors to be investigated than runs. However, this definition can be extended to the case where there are more parameters of interest than runs. They are particularly beneficial when there are a large number of parameters to investigate, but experimentation is very expensive. The idea was first introduced by Box (1959) in the discussion of Satterthwaite (1959), who suggested they be designed using random balance. Booth and Cox (1962) provided the first systematic way of constructing supersaturated designs (SSDs) when they proposed the $E(s^2)$ criterion. After many years with minimal interest in SSDs, Lin (1993) and Wu (1993) revived the topic with a construction method based on Hadamard matrices. More recent work on criteria for SSDs includes that of Jones et al. (2008) who proposed Bayesian D-optimality.

There has been very little work on using supersaturated designs to screen for interactions. Wu (1993) supplemented an SSD with interaction columns and stated that they could be used to study either the interaction or another factor. Liu et al. (2007) added interaction columns to k-circulant SSDs. However, they couldn't measure all interactions since some of the columns would be identical to each other. Lin (1998) suggested analysing main effects plans as a supersaturated design by also considering two-factor interactions.

In the vast majority of combined array and cross array experiments, some effects potentially of interest are completely confounded. This chapter illustrates how supersaturated experiments can be designed so that none of the effects of interest are completely confounded with each other, in addition to exploiting the potential for cost savings due to reduced experiment sizes. The new approach is very flexible and can deal with any number of runs and factors.

This chapter is organised as follows. Section 4.2 defines a new criterion for two-level

supersaturated experiments which is more appropriate than existing criteria when we consider the robust parameter design setting. Section 4.3 presents some examples to illustrate the benefits of the new criterion. Some further discussion is presented in Section 4.4. Tables of some new designs we generate are available on the attached CD.

4.2 Choosing supersaturated designs with control and noise factors

4.2.1 Criteria

Throughout the chapter we consider the model

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}\,, \tag{4.1}$$

where $\mathbf{Y}$ is the $n \times 1$ response vector, $\mathbf{X}$ is an $n \times p$ model matrix, $\boldsymbol{\beta}$ is a vector of p unknown coefficients and $\boldsymbol{\varepsilon}$ is a vector of independent normally distributed random errors with mean 0 and variance σ^2.

Supersaturated experiments have a necessarily complex partial aliasing structure. This results in correlated estimators of the factorial effects and can make inferring causation difficult. Thus many design construction criteria focus on trying to minimise the level of partial aliasing in a design (i.e. construct the design so that the columns of the model matrix are as near orthogonal as possible).

Suppose we were to consider only main effects in an experiment of n runs and m factors. Then $\mathbf{X}$ is an $n \times (m+1)$ model matrix. We assume that each of the m factors has two levels, coded ± 1. The first column of X is $\mathbf{1}_n = [1, \ldots, 1]^T$, with column k corresponding to the levels of the $(k-1)$th factor $(k = 2, \ldots, m+1)$. Booth and Cox (1962) proposed a criterion for two-level SSDs for m main effects that selects a design by minimising the sum of the squared inner-products between columns k and l of $\mathbf{X}$ $(k, l = 2, \ldots, m+1)$. We extend this definition to unbalanced designs and include the inner-product of the first column with every other column of $\mathbf{X}$ to give the objective function

$$E(s^2) = \frac{2}{m(m+1)} \sum_{k<l} s_{kl}^2 \,,$$

where s_{kl} is the klth element of $\mathbf{X}^{\mathrm{T}}\mathbf{X}$ $(k, l = 1, \ldots, m+1)$. Each s_{kl}^2 gives an indication of the level of partial aliasing between columns k and l, with larger values meaning stronger aliasing. This can easily be extended to the case where we wish to screen all two-factor interactions. In this case, $\mathbf{X}$ is an $n \times p$ model matrix with $p = 1 + m + m(m-1)/2$. Columns $m+2, \ldots, p$ of $\mathbf{X}$ contain the levels of the two-factor interactions between factors $k-1$ and $l-1$ $(k, l = 2, \ldots, m+1$ and $k < l)$. We have

$$E(s^2) = \frac{2}{p(p-1)} \sum_{i<j} s_{ij}^2 \,, \tag{4.2}$$

where $i, j = 1, \ldots, p$.

However, in the control by noise setting it is not particularly beneficial to estimate noise (N) main effects or noise by noise $(N \times N)$ interactions. This is because we have no control over their values in the real life process under investigation. All we are concerned about in the experiment is that they are not strongly aliased with terms that we are interested in, particularly control (C) main effects, $C \times C$ interactions and $C \times N$ interactions. Low levels of partial aliasing means that attributing observed effects to the truly active factors in the analysis is more likely.

We propose a new objective function to reflect the importance of certain effects, modifying (4.2) so that it does not take into account aliasing amongst effects which are not of interest. In general we assume there is a set $\mathcal{S}_1$ that contains the column numbers in $\mathbf{X}$ corresponding to the effects of interest and a set $\mathcal{S}_2$ which contains the column numbers corresponding to the effects which are not of interest. In a similar vein, Srivastava (1975) found *search designs* by also partitioning effects into different sets; one which the experimenter definitely wanted to estimate, one which he definitely did not, and another which may contain a relatively small number of active effects. He pointed out that the experimenter, in addition to estimating all the effects in the first set, may wish to search the final set and pick out non-negligible effects. DuMouchel and Jones (1994) partitioned effects into two groups, with those

thought likely to be active (primary) in one group and the remainder (potential) in the other.

Since those effects in $\mathcal{S}_2$ are not of any interest, we ignore inner products between their columns in a modified objective function in order to get overall more favourable aliasing amongst the terms which are of interest. We call this *effect-focussed* $E(s^2)$:

$$E_{\mathcal{S}_1}(s^2) = \frac{2}{k}\left(\sum_{i,j=1,\ldots,p;\ i<j} s_{ij}^2 - \sum_{i,j\in\mathcal{S}_2;\ i<j} s_{ij}^2\right),$$

where $k = p(p-1) - v(v-1)$ is the number of inner products corresponding to parameters of interest and v denotes the size of $\mathcal{S}_2$.

In the special case of the control by noise setting, we do not take into account inner products amongst noise main effects, $N \times N$ interactions and also between noise main effects and $N \times N$ interactions. Then we get overall more favourable aliasing amongst the terms of interest. Since, when using a supersaturated design, there are not enough runs available to estimate all effects simultaneously, we will essentially consider submodels in the analysis. Hence low levels of aliasing will also result in low bias. Jones and Nachtsheim (2009) proposed a two-part criterion, minimising the sum of the squared elements of the alias matrix, subject to a constraint on the D-efficiency of the design. In the examples they consider, there were always enough runs to be able to estimate all effects of interest, which will not be the case in this chapter.

We assume a particular ordering of the terms in the model matrix $\mathbf{X}$. Let p_C and p_N be the number of control and noise main effects. Further, let $p_{CC} = p_C(p_C-1)/2$ and $p_{NN} = p_N(p_N-1)/2$ be the number of $C\times C$ and $N\times N$ interactions. Columns $2,\ldots,p_C+1$ of $\mathbf{X}$ represent control main effects and columns $p_C+2,\ldots,p_C+p_N+2$ represent noise main effects. The following p_{CC} columns represent $C\times C$ interactions and the next $p_C p_N$ represent $C\times N$ interactions. Finally, columns $p-p_{NN}+1,\ldots,p$ represent $N\times N$ interactions. For ease of notation we define $\mathcal{S}_N = \{p_C+2,\ldots,p_C+p_N+1\}$ and $\mathcal{S}_{NN} = \{p-p_{NN}+1,\ldots,p\}$. Then $\mathcal{S}_2 = \{\mathcal{S}_N, \mathcal{S}_{NN}\}$ and the effect-focussed $E(s^2)$ objective function is as follows;

$$E_{\mathcal{S}_1}(s^2) = \frac{2}{k}\Bigg(\sum_{i,j=1,\ldots,p;\ i<j} s_{ij}^2 - \sum_{i,j\in\mathcal{S}_N;\ i<j} s_{ij}^2 - \sum_{i\in\mathcal{S}_{NN};\ j\in\mathcal{S}_N} s_{ij}^2 - \sum_{i,j\in\mathcal{S}_{NN};\ i<j} s_{ij}^2 \Bigg), \tag{4.3}$$

where $k = p(p-1) - p_N(p_N-1) - p_{NN}(p_{NN}-1) - 2p_{NN}p_N$. Notice that the second term of (4.3) excludes all the s_{ij} corresponding to inner products amongst noise main effects. The third term excludes all s_{ij} corresponding to inner products between noise main effects and $N \times N$ interactions, since we do not mind if the estimators of these effects are correlated. The fourth term excludes all s_{ij} corresponding to inner products amongst $N \times N$ interaction columns.

Although Marley and Woods (2010) showed that unbalanced supersaturated designs can achieve high power to identify active effects, it is not desirable that the designs be extremely unbalanced. Therefore it can be beneficial to give slightly more weight, $w \geq 1$, in the objective function to inner products of effects with the intercept. This can help to achieve an acceptable degree of balance in the designs, without restricting to only balanced designs. The resulting effect-focussed $E(s^2)$ criterion is

$$\text{minimise} \quad E_{\mathcal{S}_1}(s^2(w)) = \frac{2}{k}\Bigg(w \sum_{i=2,\ldots,p} s_{i1}^2 + \sum_{i,j=2,\ldots,p;\ i<j} s_{ij}^2 - \sum_{i,j\in\mathcal{S}_N;\ i<j} s_{ij}^2 - \sum_{i\in\mathcal{S}_{NN};\ j\in\mathcal{S}_N} s_{ij}^2 - \sum_{i,j\in\mathcal{S}_{NN};\ i<j} s_{ij}^2 \Bigg). \tag{4.4}$$

The first term in 4.4 gives more weight to inner products involving the intercept term. Advice on choosing w is given in Section 4.3.4. When $w = 1$, (4.4) is equivalent to minimising the objective function in (4.3). Similarly, the same benefits can be achieved by modifying (4.2) to give the intercept-weighted $E(s^2)$ criterion:

$$\text{minimise} \quad E(s^2(w)) = \frac{2}{p(p-1)}\left(w \sum_{i=2,\ldots,p} s_{i1}^2 + \sum_{i,j=2,\ldots,p;\ i<j} s_{ij}^2 \right). \tag{4.5}$$

We note that when $|\mathcal{S}_2| = 0, 1$ (4.4) and (4.5) are equivalent. When generating designs using (4.4) and (4.5) it is recommended that the maximum absolute correlation between a pair of distinct columns of interest is constrained to be below

a certain value. This will make inferring the causation of the effects easier, hence reducing the chance of type I and type II errors in the analysis. Based on previous experience we recommend that this value be 0.6. A coordinate exchange algorithm (Meyer and Nachtsheim, 1995) incorporating this constraint can be used to generate designs using (4.4) and (4.5). All designs generated in this chapter use 4,000 random starts of the algorithm. It is worth noting that if we wish to generate completely balanced designs, a columnwise algorithm (Li and Wu, 1997) could be used.

Some new designs in this chapter are also compared with those generated using the Bayesian D-optimality criterion of Jones et al. (2008). Under a Bayesian paradigm with conjugate prior distributions for $\boldsymbol{\beta}$ and σ^2 (O'Hagan and Forster, 2004), the posterior variance-covariance matrix for $\boldsymbol{\beta}$ is proportional to $(\mathbf{X}^T\mathbf{X}+\mathbf{K}/\tau^2)^{-1}$. Here, $\tau^2\mathbf{K}^{-1}$ is proportional to the prior variance-covariance matrix for $\boldsymbol{\beta}$. The resulting criterion is

$$\text{maximise} \quad D_{Bayes} = |\mathbf{X}^{\mathrm{T}}\mathbf{X} + \mathbf{K}/\tau^2|^{1/p}\,,$$

where τ^2 is a tuning parameter reflecting the available prior information. This prior information can be viewed as equivalent to having sufficient additional runs to allow estimation of all effects. Jones et al. (2008) regarded the intercept as a primary term with large prior variance, and all others as potential terms with small prior variances, see DuMouchel and Jones (1994), and set

$$\mathbf{K} = \mathbf{K}_1 = \begin{pmatrix} 0 & \mathbf{0}_{1\times(p-1)} \\ \mathbf{0}_{(p-1)\times 1} & \mathbf{I}_{(p-1)\times(p-1)} \end{pmatrix}.$$

In order to prioritise the estimation of certain terms over others, we can alter the diagonal values in the matrix $\mathbf{K}$. We give a larger prior variance to terms which are of interest by using a low value in the corresponding position in the $\mathbf{K}$ matrix. Let the ith diagonal element of $\mathbf{K}$ be denoted by k_i. For $\mathbf{K}_1$, $k_1 = 0$ and $k_i = 1$, $i = 2, \ldots, p$. Here, all terms except the intercept have equal prior variance. Suppose instead we set $k_1 = 0$, $k_i = 0.1$ for i corresponding to all terms which are of interest (i.e. those in $\mathcal{S}_1$) and $k_i = 1$ for all terms not of interest. Call this matrix $\mathbf{K}_2$. Then when using Bayesian D-optimality with $\mathbf{K}_2$, we are strongly prioritising the

estimation of effects which are of interest over those which are not.

4.3 Examples

Three detailed examples are presented to illustrate the benefits of using a SSD generated using effect-focussed $E(s^2)$. They demonstrate advantages both over other supersaturated approaches and also the more traditional methods for robust product design experiments such as combined arrays. We then briefly consider a much wider range of experiments and describe when our new criterion is most effective. In all examples we assume model (4.1).

4.3.1 Example 1: 6 control and 4 noise factors

Suppose we have six control and four noise factors. A traditional approach might use a 64-run resolution IV 2^{10-4} combined array. Russell et al. (2004) proposed a set of generating words for such an experiment. This was chosen so that the resulting design sequentially had as many clear control main effects, control by noise interactions and control by control interactions as possible. A clear effect is one which is completely free from aliasing with all other effects. However, the proposed scheme results in all control by control interactions being completely aliased with at least one other control by control interaction. Further, the array uses many more runs than is desirable for screening purposes. We demonstrate how costs can be reduced, and complete aliasing of effects of interest can be eliminated, with little impact on the correct identification of active factors. Suppose instead that we use a SSD with 28 runs, where the model matrix incorporates the intercept, all main effects and all 2-factor interactions. We generated designs using effect-focussed $E(s^2)$ and intercept-weighted $E(s^2)$ with $w = 1, 2, 4, 6$. Setting $w = 6$ produced designs which are only slightly unbalanced. For comparison, we also generated a Bayesian D-optimal design with $\mathbf{K}_1$ for 10 factors and all two-factor interactions, arbitrarily labelling the first 6 columns as control factors. Finally, a Bayesian D-optimal design with $\mathbf{K}_2$ was generated. Some of the properties of the four designs are given in Table 4.1.

Table 4.1: Properties of 28-run designs for 6 control and 4 noise factors generated using effect-focussed (E-F) $E(s^2)$-, intercept-weighted (I-W) $E(s^2)$- and Bayesian D (B-D) -optimality. Maximum absolute correlation between any pair of columns (of interest) denoted by r_{max} (r^*_{max}). Number of columns with absolute value of the column sum equal to q defined by ϕ_q.

Design	E-F ($w = 6$)	I-W ($w = 6$)	B-D ($\mathbf{K} = \mathbf{K}_1$)	B-D ($\mathbf{K} = \mathbf{K}_2$)
$E_{\mathcal{S}_1}(s^2(1))$	16.49	17.70	17.63	18.14
$E(s^2(1))$	17.60	17.28	17.27	18.33
$D_{Bayes}(\mathbf{K}_1)$	7.30	7.33	7.33	7.26
$D_{Bayes}(\mathbf{K}_2)$	3.08	3.11	3.10	3.17
r_{max}	1.00	0.50	0.58	0.58
r^*_{max}	0.50	0.50	0.58	0.58
ϕ_2	24	30	28	26
ϕ_4	2	1	5	4
ϕ_6	0	0	0	2

Notice that all four designs perform similarly well under D_{Bayes} with both $\mathbf{K}_1$ and $\mathbf{K}_2$. The Bayesian D-optimal design with $\mathbf{K}_1$ and the intercept-weighted $E(s^2)$-optimal design perform similarly well under $E(s^2(1))$ but similarly poorly under $E_{\mathcal{S}_1}(s^2(1))$, where our new design displays a clear advantage (16.49 compared to 17.70 and 17.63). The Bayesian D-optimal design with $\mathbf{K}_2$ is poor when evaluated under $E_{\mathcal{S}_1}(s^2(1))$ and $E(s^2(1))$. We denote the maximum absolute correlation between any pair of columns in the model matrix by r_{max}. Similarly, r^*_{max} denotes the maximum absolute correlation between any pair of columns of interest (that is, we excluding pairwise correlations amongst noise factor columns, amongst $N \times N$ columns and between noise factor and $N \times N$ columns). Notice that $r_{max} = 1$ for the effect-focussed $E(s^2)$-optimal design. This means that some parameters are completely aliased. However, there is no complete aliasing between any parameters which are of interest since $r^*_{max} < 1$.

We define ϕ_q as the number of columns of the model matrix with absolute value of the column sum equal to q. This can be used to indicate the degree of imbalance present in the design. We see from Table 4.1 that all four designs are slightly unbalanced, with a maximum absolute column sum of 4 for three out of the four designs, and 6 for the Bayesian D-optimal design with $\mathbf{K}_2$.

We point out that the intercept-weighted $E(s^2)$-optimal design may not be $E(s^2)$-

Table 4.2: Number of active effects in each of 10 scenarios for the simulation study for Example 1

Scenario	Main effects	$C \times C$	$C \times N$	$N \times N$
1	3	0	0	0
2	2	1	2	0
3	3	1	1	1
4	4	1	3	1
5	4	2	2	0
6	4	3	1	0
7	5	2	2	0
8	5	2	2	1
9	5	2	3	1
10	6	2	3	2

optimal due to the extra weight placed on inner products with columns involving the intercept.

To investigate the performance of the four SSDs, a simulation study was performed. This consisted of investigating 10 different scenarios of varying difficulty. Table 4.2 shows the number of active effects from each category that were present in each scenario. The scenarios range from having only a small number of active main effects, to having several active main effects along with various interactions.

Each scenario was run 1000 times with the active factors chosen at random from the relevant categories. All active factors were simulated from the distribution $N(4, 0.2)$ and all inactive factors were simulated from $N(0, 0.2)$. Data were generated from model (4.1) with error, $\boldsymbol{\varepsilon}$ from $N(0, 1)$. Note that the scenarios did not necessarily obey effect heredity.

The data were analysed using the Gauss-Dantzig selector (GDS), which was shown by Marley and Woods (2010) to be a promising analysis method for SSDs. The GDS belongs to a class of continuous variable selection techniques known as shrinkage methods, where each coefficient is shrunk towards zero at a different rate. The GDS is an extension of the original Dantzig selector method proposed by Candes and Tao (2007), where the estimator $\hat{\boldsymbol{\beta}}$ is the solution to

$$\min_{\hat{\boldsymbol{\beta}} \in \mathbb{R}^k} ||\hat{\boldsymbol{\beta}}||_1 \quad \text{subject to} \quad ||\mathbf{X}^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})||_\infty \leq \delta \,. \tag{4.6}$$

Here $||\boldsymbol{\beta}||_1 = |\beta_0| + \ldots + |\beta_m|$ is the l_1 norm, $||\boldsymbol{\beta}||_\infty = \max(|\beta_0|, \ldots, |\beta_m|)$ is the l_∞ norm, and δ is a tuning constant.

The GDS is a two-stage approach developed by Candes and Tao (2007). This was first used for the analysis of supersaturated designs by Phoa et al. (2009). Initially the Dantzig selector is used to identify the active factors, and those factors whose coefficient estimates are greater than γ are retained. Second, least squares estimates are found by regressing the response on the set of retained factors. The tuning constant γ represents the size of the smallest coefficient that would result in a factor being considered active and, in practice, could be elicited from subject experts.

To implement the GDS, we reformulate (4.6) as a linear program and solve using the package `lpSolve` (Berkelaar, 2007) in `R` (R Development Core Team, 2009). An automated selection procedure with BIC is used to choose the tuning constant δ and we set $\gamma = 1.5$. For more details see Marley and Woods (2010), Candes and Tao (2007) and Phoa et al. (2009).

We compare the designs using two summary measures;

1. *Power*; the average proportion of active factors correctly identified. This is a larger-the-better measure.

2. *Type I error rate*; the average proportion of inactive factors which are declared active. This is a smaller-the-better measure.

Since we are only interested in certain effects, power is divided into power for C, N, $C \times C$, $C \times N$ and $N \times N$ effects. Type I error rate is considered only for C main effects, $C \times C$ and $C \times N$ interactions combined.

Power for different effects and Type I error rate for the effect-focussed $E(s^2)$-optimal design is given in Table 4.3. The corresponding figures for the intercept-weighted $E(s^2)$-optimal design are shown in Table 4.4, and for the Bayesian D-optimal designs with $\mathbf{K}_1$ and $\mathbf{K}_2$ in Tables 4.5 and 4.6. An NA in a table means that a particular effect was not present in the given scenario.

Table 4.3: Powers for various effects and Type I error rate for the 28-run design for Example 1 generated using effect-focussed $E(s^2)$ with $w = 6$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.97	NA	NA	NA	0.01
2	0.99	0.92	0.98	0.99	NA	0.02
3	0.98	0.89	0.95	0.98	0.50	0.02
4	0.93	0.86	0.83	0.89	0.45	0.05
5	0.94	0.90	0.89	0.93	NA	0.04
6	0.93	0.89	0.87	0.92	NA	0.04
7	0.92	0.87	0.84	0.88	NA	0.05
8	0.88	0.82	0.79	0.86	0.42	0.06
9	0.84	0.80	0.74	0.80	0.39	0.07
10	0.79	0.73	0.68	0.75	0.36	0.10

Table 4.4: Powers for various effects and Type I error rate for the 28-run design for Example 1 generated using intercept-weighted $E(s^2)$ with $w = 6$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	1.00	NA	NA	NA	0.01
2	0.97	0.98	0.97	0.97	NA	0.02
3	0.95	0.94	0.91	0.96	0.94	0.03
4	0.85	0.86	0.81	0.84	0.83	0.06
5	0.90	0.91	0.86	0.88	NA	0.04
6	0.89	0.91	0.86	0.88	NA	0.05
7	0.85	0.88	0.82	0.83	NA	0.06
8	0.82	0.83	0.77	0.80	0.78	0.07
9	0.74	0.76	0.69	0.73	0.74	0.09
10	0.67	0.67	0.58	0.66	0.65	0.12

Table 4.5: Powers for various effects and Type I error rate for the 28-run design for Example 1 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_1$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.99	NA	NA	NA	0.01
2	0.96	0.97	0.98	0.97	NA	0.02
3	0.94	0.96	0.94	0.95	0.96	0.03
4	0.81	0.85	0.82	0.83	0.83	0.06
5	0.89	0.87	0.86	0.89	NA	0.05
6	0.89	0.85	0.86	0.88	NA	0.05
7	0.84	0.85	0.80	0.82	NA	0.06
8	0.78	0.79	0.77	0.79	0.79	0.08
9	0.74	0.74	0.72	0.75	0.73	0.09
10	0.65	0.65	0.59	0.67	0.66	0.13

Table 4.6: Powers for various effects and Type I error rate for the 28-run design for Example 1 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_2$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.99	NA	NA	NA	0.01
2	0.97	0.92	0.97	0.97	NA	0.02
3	0.94	0.90	0.93	0.94	0.88	0.03
4	0.86	0.75	0.87	0.84	0.70	0.06
5	0.91	0.80	0.89	0.89	NA	0.04
6	0.91	0.82	0.86	0.90	NA	0.04
7	0.87	0.76	0.83	0.84	NA	0.06
8	0.83	0.71	0.80	0.80	0.66	0.08
9	0.76	0.62	0.75	0.73	0.59	0.09
10	0.68	0.54	0.69	0.66	0.48	0.12

Notice from Tables 4.3-4.6 that the effect-focussed $E(s^2)$-optimal design always beats the intercept-weighted $E(s^2)$- and Bayesian D-optimal (with $\mathbf{K}_1$) designs under power for C main effects, $C \times C$ and $C \times N$ interactions which indicates the clear benefits of our new criterion over existing criteria for SSDs. We also see comparable or even more favourable Type I error rates for our new design. Notice that power for $N \times N$ interactions is particularly low for the effect-focussed $E(s^2)$-optimal design due to some of these effects being completely aliased with each other. However, since we cannot control these effects in practice, we accept the trade off of better identifiability of C main effects, $C \times C$ and $C \times N$ interactions. The effect-focussed $E(s^2)$-optimal design also outperforms the Bayesian D-optimal design with $\mathbf{K}_2$ under power for C main effects and $C \times N$ interactions and Type I error rate, whilst performing similarly under power for $C \times C$ interactions.

Notice that as we increase the number of active effects, the powers tend to decrease and Type I error rates increase. This is in line with an observation of Marley and Woods (2010). However, for the effect-focussed $E(s^2)$-optimal design, the power is still very high, even for scenario 8, which has a relatively large number of active main effects (five) and interactions (five). This is achieved using only 28 runs - considerably less than the 64 runs that may have been used in the traditional combined array approach, and without the complete aliasing of effects of interest.

4.3.2 Example 2: 4 control and 6 noise factors

Now consider an experiment with 4 control and 6 noise factors. In this case, we would expect to see considerable benefits from using effect-focussed $E(s^2)$-optimality, since we have more noise factors than control factors. Therefore, we are able to sacrifice good aliasing between many effects in order to achieve more desirable aliasing between effects of interest. As in Example 1, we generate SSDs using effect-focussed $E(s^2)$ and intercept-weighted $E(s^2)$ with $w = 1, 2, 4, 6$ and also Bayesian D-optimality with $\mathbf{K}_1$ and $\mathbf{K}_2$. The designs all have 24 runs. In this instance, setting $w = 4$ produced designs which achieved a reasonable degree of balance. Some of the properties of the four designs are given in Table 4.7.

Notice that the effect-focussed $E(s^2)$-optimal design has a much lower value of

Table 4.7: Properties of 24-run designs for 4 control and 6 noise factors generated using effect-focussed (E-F) $E(s^2)$-, intercept-weighted (I-W) $E(s^2)$- and Bayesian D (B-D) -optimality. Maximum absolute correlation between any pair of columns (of interest) denoted by r_{max} (r^*_{max}). Number of columns with absolute value of the column sum equal to q defined by ϕ_q.

Design	E-F ($w = 4$)	I-W ($w = 4$)	B-D ($\mathbf{K} = \mathbf{K}_1$)	B-D ($\mathbf{K} = \mathbf{K}_2$)
$E_{\mathcal{S}_1}(s^2(1))$	10.43	16.15	16.49	16.43
$E(s^2(1))$	18.83	16.02	16.02	19.11
$D_{Bayes}(\mathbf{K}_1)$	5.39	5.53	5.53	5.39
$D_{Bayes}(\mathbf{K}_2)$	2.83	2.79	2.86	2.95
r_{max}	1.00	0.58	0.58	1.00
r^*_{max}	0.44	0.58	0.58	0.58
ϕ_2	22	28	27	18
ϕ_4	8	2	0	8
ϕ_6	6	0	1	0
ϕ_8	0	0	0	4

$E_{\mathcal{S}_1}(s^2(1))$ than the other three designs. It also has a lower value of r^*_{max} and again displays complete aliasing between some effects which are not of interest. For this example, the Bayesian D-optimal design with $\mathbf{K}_2$ also displays complete aliasing, and also has the most unbalanced columns of all the designs ($\phi_8 = 4$).

As in Section 4.3.1, the four designs were compared by way of a simulation study. Similar scenarios to those in Section 4.3.1 were used, and are detailed in Table 4.8. Each scenario was run and analysed in the same way as 4.3.1.

Power for different effects and Type I error rate for the effect-focussed $E(s^2)$-optimal design is given in Table 4.9. The corresponding figures for the intercept-weighted $E(s^2)$-optimal design are shown in Table 4.10, and for the Bayesian D-optimal designs with $\mathbf{K}_1$ and $\mathbf{K}_2$ in Tables 4.11 and 4.12.

Notice that we see large improvements in power for C main effects, $C \times C$ interactions and $C \times N$ interactions for the effect-focussed $E(s^2)$-optimal design. For example, for scenario 5, where there are 4 active main effects and 4 active interactions, the powers for C main effects, and $C \times N$ interactions are 0.95 and 0.94. This compares to only 0.78 and 0.72 for the intercept-weighted $E(s^2)$-optimal design. Similarly, the Type I error rate for this scenario is only 0.03 for the effect-focussed $E(s^2)$-optimal design compared to 0.07 for the intercept-weighted $E(s^2)$-optimal design. It is also

Table 4.8: Number of active effects in each of 10 scenarios for the simulation study for Example 2

Scenario	Main effects	$C \times C$	$C \times N$	$N \times N$
1	3	0	0	0
2	2	0	2	1
3	3	1	1	1
4	4	1	3	1
5	4	0	2	2
6	4	0	1	3
7	5	0	2	2
8	5	1	2	2
9	5	1	3	2
10	6	2	3	2

Table 4.9: Powers for various effects and Type I error rate for the 24-run design for Example 2 generated using effect-focussed $E(s^2)$ with $w = 4$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.64	NA	NA	NA	0.01
2	0.97	0.60	NA	0.97	0.21	0.02
3	0.98	0.57	0.94	0.97	0.19	0.02
4	0.88	0.56	0.81	0.87	0.17	0.06
5	0.95	0.53	NA	0.94	0.17	0.03
6	0.97	0.51	NA	0.95	0.16	0.03
7	0.94	0.52	NA	0.92	0.17	0.04
8	0.90	0.52	0.79	0.85	0.16	0.06
9	0.85	0.50	0.73	0.80	0.16	0.08
10	0.76	0.48	0.66	0.70	0.14	0.11

Table 4.10: Powers for various effects and Type I error rate for the 24-run design for 4 Example 2 generated using intercept-weighted $E(s^2)$ with $w = 4$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	0.99	0.99	NA	NA	NA	0.02
2	0.92	0.90	NA	0.89	0.93	0.03
3	0.90	0.86	0.82	0.86	0.83	0.04
4	0.71	0.71	0.63	0.66	0.66	0.08
5	0.78	0.79	NA	0.72	0.73	0.07
6	0.78	0.79	NA	0.75	0.71	0.06
7	0.74	0.73	NA	0.67	0.67	0.08
8	0.69	0.69	0.56	0.61	0.61	0.09
9	0.63	0.63	0.51	0.55	0.57	0.11
10	0.57	0.55	0.47	0.50	0.49	0.13

Table 4.11: Powers for various effects and Type I error rate for the 24-run design for Example 2 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_1$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	0.99	0.98	NA	NA	NA	0.02
2	0.91	0.88	NA	0.91	0.89	0.03
3	0.85	0.83	0.85	0.84	0.82	0.04
4	0.68	0.67	0.68	0.67	0.65	0.09
5	0.72	0.73	NA	0.71	0.71	0.08
6	0.73	0.75	NA	0.69	0.70	0.08
7	0.69	0.71	NA	0.64	0.62	0.09
8	0.63	0.63	0.62	0.61	0.58	0.11
9	0.59	0.59	0.58	0.57	0.56	0.12
10	0.53	0.51	0.50	0.52	0.49	0.14

Table 4.12: Powers for various effects and Type I error rate for the 24-run design for Example 2 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_2$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	0.98	0.63	NA	NA	NA	0.02
2	0.92	0.55	NA	0.92	0.52	0.03
3	0.93	0.54	0.98	0.87	0.49	0.04
4	0.82	0.42	0.88	0.76	0.34	0.09
5	0.84	0.47	NA	0.79	0.41	0.07
6	0.80	0.48	NA	0.79	0.40	0.07
7	0.78	0.44	NA	0.75	0.35	0.09
8	0.76	0.43	0.88	0.72	0.37	0.10
9	0.75	0.40	0.85	0.69	0.31	0.12
10	0.69	0.35	0.78	0.60	0.27	0.15

worth noting the consistently high powers, especially for scenarios 1-8, despite the fact that we are using a design with only 24 runs.

Using $\mathbf{K}_2$ instead of $\mathbf{K}_1$ in the Bayesian D-optimality criterion results in a design with higher power for effects of interest. However, neither design beats the performance of the effect-focussed $E(s^2)$-optimal design.

4.3.3 Example 3: 5 control and 3 noise factors

In this section we present an example with 5 control and 3 noise factors. Miller et al. (1993) considered an experiment with the same number of factors where two replicates of a 128-run cross array were used. Here, we apply our new methods to construct experiments with only 20 runs, and demonstrate how they may perform in practice. This example also illustrates that higher power for effects of interest can still be achieved by using effect-focussed $E(s^2)$-optimality, despite there only being a relatively small number of noise factors and noise by noise interactions. The same procedure as for Examples 1 and 2 was followed, with four SSDs being generated. Some of the properties of the four designs are given in Table 4.13.

In this case, the effect-focussed $E(s^2)$-, intercept-weighted $E(s^2)$- and Bayesian D-optimal ($\mathbf{K}_1$) designs perform similarly under $E(s^2(1))$ and $D_{Bayes}(\mathbf{K}_1)$. However, the intercept weighted $E(s^2)$- and Bayesian D-optimal designs do considerably worse

Table 4.13: Properties of 20-run designs for 5 control and 3 noise factors generated using effect-focussed (E-F) $E(s^2)$-, intercept-weighted (I-W) $E(s^2)$- and Bayesian D (B-D) -optimality. Maximum absolute correlation between any pair of columns (of interest) denoted by r_{max} (r^*_{max}). Number of columns with absolute value of the column sum equal to q defined by ϕ_q.

Design	E-F ($w = 6$)	I-W ($w = 6$)	B-D ($\mathbf{K} = \mathbf{K}_1$)	B-D ($\mathbf{K} = \mathbf{K}_2$)
$E_{\mathcal{S}_1}(s^2(1))$	10.49	12.39	12.39	12.71
$E(s^2(1))$	12.18	12.18	12.16	12.72
$D_{Bayes}(\mathbf{K}_1)$	6.86	6.86	6.87	6.81
$D_{Bayes}(\mathbf{K}_2)$	3.01	3.06	3.07	3.15
r_{max}	1.00	0.41	0.50	0.50
r^*_{max}	0.41	0.41	0.50	0.50
ϕ_2	0	0	8	13
ϕ_4	4	3	1	1
ϕ_6	0	0	0	1
ϕ_8	0	0	0	1

Table 4.14: Number of active effects in each of 8 scenarios for the simulation study for Example 3

Scenario	Main effects	$C \times C$	$C \times N$	$N \times N$
1	3	0	0	0
2	2	2	0	0
3	2	0	1	0
4	2	2	1	0
5	2	0	0	2
6	2	0	1	1
7	3	1	1	1
8	4	1	2	2

than the effect-focussed $E(s^2)$ design when evaluated under $E_{\mathcal{S}_1}(s^2(1))$. All designs have reasonably low r^*_{max}. Again, the Bayesian D-optimal design with $\mathbf{K}_2$ is the most unbalanced. This time eight different simulation scenarios are considered (shown in Table 4.14).

The simulation was performed as in Sections 4.3.1 and 4.3.2. Power for different effects and Type I error rate for the design generated using effect-focussed $E(s^2)$ is given in Table 4.15. The corresponding figures for the designs generated using intercept-weighted $E(s^2)$ and Bayesian D-optimality are shown in Tables 4.16, 4.17 and 4.18.

Table 4.15: Powers for various effects and Type I error rate for the 20-run design for Example 3 generated using effect-focussed $E(s^2)$ with $w = 4$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.95	NA	NA	NA	0.02
2	0.98	0.93	0.98	NA	NA	0.03
3	0.99	0.93	NA	1.00	NA	0.02
4	0.95	0.90	0.96	0.95	NA	0.04
5	1.00	0.64	NA	NA	0.03	0.02
6	0.99	0.79	NA	0.99	0.04	0.02
7	0.96	0.80	0.94	0.95	0.04	0.04
8	0.87	0.63	0.85	0.84	0.04	0.08

Table 4.16: Powers for various effects and Type I error rate for the 20-run design for Example 3 generated using intercept-weighted $E(s^2)$ with $w = 4$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	1.00	NA	NA	NA	0.02
2	0.98	0.96	0.98	NA	NA	0.02
3	0.99	1.00	NA	0.99	NA	0.02
4	0.96	0.94	0.95	0.93	NA	0.03
5	0.98	0.98	NA	NA	0.97	0.03
6	0.97	0.99	NA	0.96	0.97	0.03
7	0.93	0.93	0.88	0.88	0.86	0.05
8	0.76	0.79	0.65	0.69	0.66	0.13

Table 4.17: Powers for various effects and Type I error rate for the 20-run design for Example 3 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_1$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	0.99	1.00	NA	NA	NA	0.02
2	0.99	0.96	0.98	NA	NA	0.03
3	0.99	0.99	NA	0.99	NA	0.02
4	0.96	0.94	0.96	0.92	NA	0.04
5	0.98	0.99	NA	NA	0.98	0.03
6	0.98	0.97	NA	0.97	0.98	0.02
7	0.92	0.88	0.88	0.87	0.90	0.05
8	0.74	0.74	0.70	0.69	0.73	0.12

Table 4.18: Powers for various effects and Type I error rate for the 20-run design for Example 3 generated using Bayesian D-optimality with $\mathbf{K} = \mathbf{K}_2$

Scenario	Power					Type I error rate
	C	N	$C \times C$	$C \times N$	$N \times N$	
1	1.00	0.98	NA	NA	NA	0.02
2	0.98	0.96	0.99	NA	NA	0.02
3	0.98	0.96	NA	0.98	NA	0.02
4	0.96	0.95	0.98	0.95	NA	0.03
5	0.91	0.95	NA	NA	0.88	0.03
6	0.95	0.92	NA	0.96	0.90	0.03
7	0.90	0.86	0.94	0.87	0.77	0.05
8	0.71	0.67	0.80	0.70	0.53	0.13

It can be seen that for scenarios 1-4, the four designs perform similarly, with very high powers for C main effects, $C \times C$ interactions and $C \times N$ interactions and similar Type I error rates. However, for scenarios 5-8 the effect-focussed $E(s^2)$-optimal design has higher power for C main effects, $C \times C$ interactions and $C \times N$ interactions and also a lower Type I error rate. Thus using our new criterion can be beneficial even when there are only a small number of noise factors. The powers for scenarios 1-7 are all very high, indicating how successful a supersaturated design can be. This design also has the benefit of having 12 fewer runs than a more traditional 32 run combined array, thus dramatically reducing experimental cost.

4.3.4 Other examples

Examples 1, 2 and 3 illustrate how the new effect-focussed $E(s^2)$-optimality criterion can produce designs which perform better in practice than other supersaturated approaches. They also demonstrate how high power and low Type I error rate for effects of interest can be achieved in only a small number of runs. Many other examples for p_C and p_N ranging from 3 to 6 and varying run sizes were investigated and trends following those seen in Examples 1, 2 and 3 were observed. The largest gains from using effect-focussed $E(s^2)$ were seen when the number of noise factors was greater than the number of control factors, which is to be expected.

Throughout the chapter, only two different $\mathbf{K}$ matrices have been used to generate designs. These have $k_i = 1$ or $k_i = 0.1$ for i corresponding to terms in $\mathcal{S}_1$. We also

generated a selection of designs using $k_i = 0.5$ and $k_i = 0.01$ for $i \in \mathcal{S}_1$ but found that results for the designs with $k_i = 0.1$ gave overall better results than $k_i = 0.5$ or $k_i = 0.01$.

Let $t = p_C + p_C(p_C - 1)/2 + p_C p_N + 1$ be the total number of parameters of interest. For $t < n < p$ the number of parameters of interest is less than the number of runs, but the design is still supersaturated relative to the total number of parameters. In this situation, when generating a Bayesian D-optimal design it is possible to set $k_i = 0$ for each parameter of interest, that is, making each parameter of interest a *primary* term. However, for many combinations of control and noise factors the number of runs required to be able to do this is often larger than the experimenter would have at his disposal, given that he is considering performing a supersaturated experiment. Nevertheless, if such an experiment were to be performed, simulation results (not presented) have shown that all the criteria produce designs which are very effective in a screening situation, since the designs are only marginally supersaturated, with p/n typically only slightly greater than 1. In situations where p/n is a little larger, for instance in Example 2 with $n = 38$, the effect-focussed $E(s^2)$-optimal design still performs the best out of all approaches considered.

It should be mentioned that effect-focussed $E(s^2)$ and intercept-weighted $E(s^2)$ in particular are not trivial to optimise. Many random starts of the coordinate exchange algorithm are required and even then, the solution is not guaranteed to be optimal.

Another task for the experimenter is choose which value of w to use. As in the three examples presented, we recommend generating designs for different values of w and then picking the most appropriate design for the given experiment based on the design properties. Some experimenters may not desire a large number of unbalanced columns and hence in general they will need to choose a higher w. However, other experimenters may be more willing to accept more unbalanced columns in return for slightly better aliasing amongst effects of interest.

4.4 Discussion

It has been demonstrated that the use of SSDs in a robust product design setting can be very effective. A new *effect-focussed* $E(s^2)$ criterion to reflect the importance of estimating certain effects has been proposed and shown to be successful. This criterion reduces to the standard $E(s^2)$ criterion in the case where there are no noise variables. There are two main benefits over existing approaches;

1. No complete aliasing between effects of interest.
2. The ability to achieve high power and low Type I error rates for effects of interest in a relatively small number of runs.

When using a SSD, it is important to choose a run size that enables identification of active effects with high probability. Power to detect active effects depends not only on run size but also on variables such as the number and magnitude of active effects and the error variance. However, examining the results of all simulation studies performed across a wide range of examples and scenarios, we can make the following recommendation;

$$\text{The minimum run size should be at least } \frac{1}{2}\left(t + (p-t)/2\right) ,$$

where t is the total number of parameters of interest. This should enable the detection of most moderate-sized effects (see also the recommendations of Marley and Woods, 2010).

The benefits of using effect-focussed $E(s^2)$ will be strongest when there is a reasonable number of noise variables relative to control variables. This means that there are enough N main effects and $N \times N$ interactions relative to the total number of parameters for effect-focussed $E(s^2)$ to make a large difference over intercept-weighted $E(s^2)$ in terms of practical performance. However, examples have shown that even when there are considerably more control factors than noise factors, there are still clear benefits of using effect-focussed $E(s^2)$.

We also make a comment on the flexibility of our method. Since our new designs are generated by the coordinate exchange algorithm, it is possible, for a sensible number of C and N main effects, to generate designs for any number of runs.

We mention that it may not always be desirable to perform a robust product design experiment which places no emphasis on screening noise main effects or noise by noise interactions. In some circumstances, the experimenter may be required to produce recommended settings for the noise factors. In such cases, the effect-focussed $E(s^2)$ criterion proposed in this chapter would not be suitable. However, if the experimenter has no control whatsoever over the noise factors then we strongly recommend the use of effect-focussed $E(s^2)$-optimality.

Finally, we note that supersaturated designs are typically the first step in a sequence of experiments and help to establish which control by noise interactions have the potential to dampen the effect of variation in the noise factors. Subsequent experiments may be required to determine the precise settings of the control factors which achieve this aim, and such experiments may require different subsets of factorial effects to be emphasised (for instance the main effects of the noise factors). Effect-focussed $E(s^2)$ designs for these different sets of effects may then be usefully employed.

We point out that follow-up runs may also be required in more traditional combined array approaches in order to de-alias effects of interest which are fully confounded.

Chapter 5

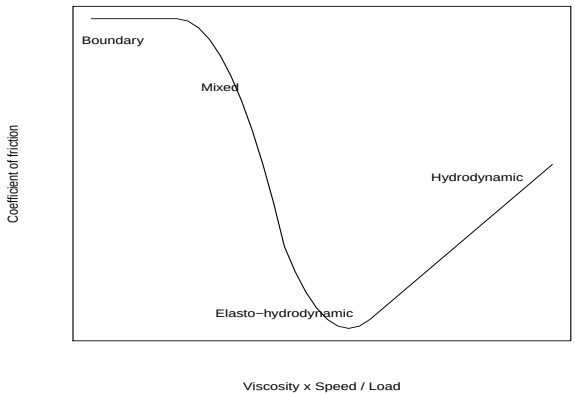
Advancing Tribology: Designed experiments to investigate the impact of oil properties and process variables on friction

The statistical methodology behind an experiment in tribology to investigate the effect of factors on the shape of Stribeck curves is presented. We describe the techniques developed to design an experiment where the levels of some of the factors cannot be set directly. We also describe the two-stage analysis of the data from the experiment, where the output from each run was a set of points forming a curved relationship, known in tribology as a Stribeck curve. Principal component analysis was first performed to obtain a common form for each curve, and then a linear model was fitted to relate principal component loadings to the factor levels. To follow-up on findings from the initial experiment, new methodology is developed for choosing additional design points for such a two-stage model. In addition to the methodology, we present conclusions about which factors are having the substantial effects, and how they influence the shape of the Stribeck curve.

5.1 Introduction

Tribology is the study of interacting surfaces in relative motion. In order to reduce friction between two surfaces which are rubbing against each other, oil can be placed between the surfaces involved. This can result in greater efficiency in a system, for

Figure 5.1: Characteristic form of the Stribeck curve, showing how coefficient of friction relates to speed, load and viscosity. Different lubrication regimes are labeled.

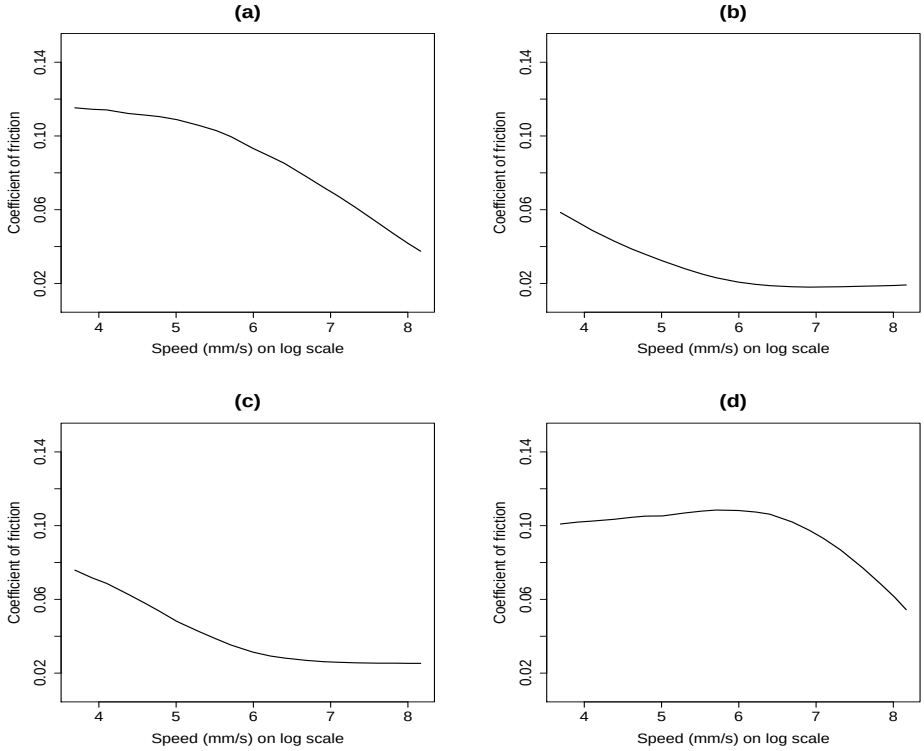


example less wear of components in a gearbox or the smoother running of parts in an engine. Friction is often measured by the *coefficient of friction*; a number which represents the friction between two surfaces. Stribeck (1902) presented the first work studying how the coefficient of friction varied with speed, load and viscosity. The characteristic form of this relationship became known as the *Stribeck curve* (see Dowson, 1998, pp 344-345) and is shown in Figure 5.1.

Although Figure 5.1 gives the general form of the Stribeck curve, observed Stribeck curves may vary depending on experimental conditions. In particular, different properties of the oil used, or different settings for certain process variables, may change the shape of observed Stribeck curves to varying degrees. For example, Figure 5.2 shows four different Stribeck curves obtained from a test procedure using different oils and different levels of two process variables. The curves are displayed as function of speed. Further details about the test procedure are given in Section 5.2.1. Notice that curves (a) and (d) are very different from (b) and (c). We also see more subtle differences, for instance between curves (a) and (d). Curve (d) appears to have peaked at around log(speed) = 6, whereas curve (a) displays no turning point.

It is useful for tribologists to be able to model the shape of the Stribeck curve and establish which variables are having an impact on the shape of the curve and the form of this relationship. This information is particularly useful when investigating variables that can be controlled in product development, as when developing a

Figure 5.2: Four example Stribeck curves obtained using different oils and different settings of process variables



suitable oil to lubricate surfaces. The Stribeck curve is useful not only for establishing the coefficient of friction, but also for determining when the system enters different lubrication regimes, as indicated in Figure 5.1. Systems may require different lubricants in different regimes. Figure 5.1 indicates that the curves in Figure 5.2 (a) and (d) are in the boundary/mixed region, whilst (b) and (c) are in the mixed/elasto-hydrodynamic region.

Recent work, for instance Lu et al. (2006) and Sojoudi and Khonsari (2010), focussed on theoretical models for Stribeck curves. One of the drawbacks of these theoretical models is that they are not expressed in terms of directly controllable variables, which limits their application.

In this chapter we describe the methodology behind a series of studies to investigate the impact of different oils and process variables on the shape of Stribeck curves. The empirical models we use were constructed from the output of designed experiments run by The Lubrizol Corporation, who were particularly interested in how certain variables influenced the shape of the observed Stribeck curve. We consider both the

design of the studies and the analysis of the resulting data. In total, 30 runs of a test procedure were performed to give a total of 30 observed Stribeck curves from which to construct a model. The 30 runs were split into a screening stage of 20 runs to identify the important factors and then a follow-up stage of 10 runs to enable a more precise model to be estimated, and to follow up on important effects. To design the follow-up experiment, new methods are presented for the optimal design for two-stage mixed models.

The set-up of the experimental design is particularly novel, due to the fact that not all of the factor levels can be set directly. Some of the factors are in fact linear combinations of the ingredients added to a base oil (see Section 5.2 for further details). As a consequence, standard criteria and algorithms need to be adapted accordingly.

The analysis of the resulting data is challenging due to each response being an observed Stribeck curve as opposed to a single data point. For each experimental run, we obtain 21 data points, which when interpolated form part of the curve shown in Figure 5.1. A two-stage semi-parametric procedure was used to model the data, with the models for the curves first being constructed in terms of the principal components (PCs; see for instance Ramsay and Silverman, 2005, ch. 8). In the second stage, the PC loadings were then related to the factors. A similar two-stage approach was taken by Grove et al. (2004) who discussed a case study involving engine mapping in the automotive industry and by Aston et al. (2010) who constructed a quantitative model for pitch in the spoken language Luobuzhai Qiang.

The remainder of this chapter is organised as follows. Section 5.2 briefly details the test procedure used and discusses the design of the initial experiment. We also present a brief description of the factors included in the experiment. Section 5.3 presents the two-stage analysis of the data. We describe a novel procedure for obtaining follow-up runs in Section 5.4, and present the final fitted model in Section 5.5. Some further discussion and concluding remarks are given in Section 5.6.

5.2 Obtaining the data

This section gives brief details of the test procedure for the experiment and also the machine on which it is run. We also discuss the factors which were varied in the experiment and how several of them are determined from proportions of ingredients which are added to a base oil. Finally, we describe how a 20-run experiment was designed, including adaptations of an existing algorithm and criterion to incorporate the factors where the levels could not be directly set.

5.2.1 The test procedure

Lubrizol ran the experiments on a Mini Traction Machine (MTM). This involved a ball rotating against a spinning disc for approximately 6 hours. Lubricating oil was placed between the ball and the disc before the start of each run. A different disc and ball surface was used for each run. The Stribeck curve was obtained by slowly reducing the speed of the disc at the end of the experiment. Measurements of the coefficient of friction were obtained automatically by the MTM for 21 speeds per run. The Stribeck curves can then be displayed as a plot of coefficient of friction against log(speed), as in Figure 5.2.

5.2.2 Factors to be varied

The collaborating company were interested in how a total of thirteen factors affected the shape of the Stribeck curve. Two of these were process variables (disc roughness and load on the disc), whilst the others were properties of the oil used to lubricate the disc. The factors are listed in Table 5.1, split into process variables and characteristics. Characteristics are quantitative variables describing properties of the oil.

Load and roughness could be set at two possible levels. The high level for load was 72N and the low level was 37N. The two levels of roughness were categorised as 'rough' and 'smooth'. The differences between the rough and smooth discs in terms of R_a and R_{sk} (two recognised measures of roughness) were substantial. R_a is defined as the average absolute deviation from the mean line of the measurements in a

Table 5.1: Factors to be varied in the Stribeck curve experiment

Characteristics	Process variables
1. ZN_APHOS	12. Load
2. ZN_PPHOS	13. Disc roughness
3. ZN_SPHOS	
4. Phosphate Phos	
5. Dispersant nitrogen (Disp N)	
6. Dispersant boron (Disp B)	
7. Detergent calcium (Det CA)	
8. Detergent magnesium (Det MG)	
9. Detergent total base number (Det TBN)	
10. Inclusion of an extreme pressure (EP) additive	
11. Inclusion of a friction modifier (FM)	

roughness profile taken by running a stylus across a portion of the disc. Similarly R_{sk} is the skewness of the profile measurements. The rough discs used in the experiment were chosen from a larger batch to be as similar to each other as possible in terms of these measurements; the smooth discs were chosen similarly. Measures of roughness are discussed further in Section 5.6.

The majority of the characteristics to be varied in the experiment cannot be set directly. They are in fact functions of the proportions of various different ingredients in the oil. Each oil is made up of a large amount of base oil (typically over 90%) and then a small amount of other ingredients or 'additives'. Each of these ingredients is described by a set of characteristics, which are some of the factors to be investigated. Generics are then constructed as the weighted sum of the characteristic values, with the weights being the proportion of each ingredient in the oil. The factor levels in the design are the generics after scaling to the region [-1,1]. Generics are regularly used by the company to model the effect of oil properties.

There were eleven different ingredients which are described by the eleven characteristics in Table 5.1. Their characteristic values are given in Table 5.2.

Notice how the characteristic matrix in Table 5.2 is in blocks. This is because certain characteristics relate only to certain classes of ingredients, for example detergents or dispersants.

As an example of how the generics are calculated, consider the generic for Det CA

Table 5.2: Characteristic values for eleven ingredients

Ingredient/Characteristic	ZN_APHOS	ZN_PPHOS	ZN_SPHOS	Phosphate Phos	Disp N	Disp B	Det CA	Det MG	Det TBN	Inclusion of EP	Inclusion of FM
ZDP1	0	9.5	0	0	0	0	0	0	0	0	0
ZDP2	0	0	10	0	0	0	0	0	0	0	0
ZDP3	3.2	0	0	0	0	0	0	0	0	0	0
Antiwear	0	0	0	8.5	0	0	0	0	0	0	0
Dispersant 1	0	0	0	0	2.3	1.9	0	0	0	0	0
Dispersant 2	0	0	0	0	1.16	0	0	0	0	0	0
Detergent 1	0	0	0	0	0	0	15.5	0.04	400	0	0
Detergent 2	0	0	0	0	0	0	12	0	300	0	0
Detergent 3	0	0	0	0	0	0	0.05	9.4	400	0	0
EP1	0	0	0	0	0	0	0	0	0	1	0
FM1	0	0	0	0	0	0	0	0	0	0	1

if we use 2% of Detergent 1 and 1% of Detergent 2 in the oil. Then we have

$$\text{Generic for Det CA} = 0.02 \times 15.5 + 0.01 \times 12 = 0.43$$

For ease of notation, we let $\mathbf{C}$ be the $a \times c$ matrix of values of c characteristics for a ingredients. We also let $\mathbf{W}$ be a $n \times a$ matrix containing the proportions of each ingredient in the overall blend for each of the n runs in the experiment. Then the $n \times c$ matrix of generics for the experiment is given by $\mathbf{WC}$. In the example we consider, $a = 11$, $c = 11$ and $n = 20$ for the first experiment.

We note that the values of the characteristics EP and FM could, in fact, be set directly, since they are simply amounts of one ingredient and there are no constraints on them except for a maximum permitted amount for inclusion. However, we include them in the matrix $\mathbf{C}$ in keeping with the other characteristics. This will aid description and implementation of the design generation method.

5.2.3 Designed experiment

In designing an experiment, we have to pick the amounts (or weights) of each ingredient to use for each run, along with the appropriate levels of load and roughness so that the 20 runs available at the first stage of the experiment provide good information about the effect of varying the generics and other factor levels on the coefficient of friction.

We notice that some of the characteristics in Table 5.2 are correlated. Therefore it will not be possible to obtain an orthogonal design. We also have several constraints which must be adhered to in the design.

1. There are maximum and minimum amounts of each ingredient that can be used (see Table 5.3).

2. Despite twenty runs being available, due to cost constraints only twelve different oils can be used (i.e., only twelve different combinations of generics for characteristics 1-11). However, different settings of the two process variables can be used for runs with the same oil.

Table 5.3: Minimum and maximum percentages of the eleven ingredients in the oils

Ingredient	Min %	Max %
ZDP1	0	0.42
ZDP2	0	0.40
ZDP3	0	0.48
Antiwear	0	0.47
Dispersant 1	0	2
Dispersant 2	0	4
Detergent 1	0	3
Detergent 2	0	3
Detergent 3	0	3
EP	0	0.1
FM	0	0.1

3. Characteristics 1-4 each represent an amount of a different type of phosphorous. The total amount of phosphorous in any oil used must be between 0.01 and 0.04%.

4. Only one of the three ZDP ingredients and one of the two dispersants can be used in a given oil.

Strictly speaking, each oil used in the experiment is a mixture, with the ingredients in Table 5.3 making up a certain proportion of the overall oil. The remainder of the oil is made up of base oil. Since base oil makes up over 90% of each mixture, the system can be studied by designing the experiment and constructing the model ignoring the mixture constraints (see Snee, 1973). The large percentage component (i.e. the base oil) is known as the slack variable. An increase or decrease in one of the ingredients in Table 5.2 is achieved by a corresponding decrease or increase in the slack variable.

The criterion we use use for designing the experiment is D-optimality, which maximises

$$\phi_D^{(1)} = |\mathbf{X}^T\mathbf{X}|\,, \tag{5.1}$$

where $|\mathbf{A}|$ denotes the determinant of $\mathbf{A}$. The model matrix is denoted by $\mathbf{X}$. In this experiment, it was decided to focus investigation primarily on the main effects

of the factors. However a check on the resulting design was performed to ensure that two-factor interactions were also estimable to allow investigation of these effects if necessary. Therefore, the model matrix is given by

$$\mathbf{X} = [\mathbf{1}|\mathbf{WC}|\mathbf{P}],$$

where $\mathbf{P}$ is the 20×2 design matrix for the two process variables and $\mathbf{1}$ is a 20×1 column of 1s. The optimisation is with respect to $\mathbf{W}$ and $\mathbf{P}$.

Because of the nature of the constraints, it was decided that a form of exchange algorithm was appropriate to generate the design. A candidate list of weights for the weight matrix $\mathbf{W}$ was constructed that incorporated the 'extreme' vertices of the eleven characteristics under investigation. This was a suitable candidate list to use, as D-optimality tends to push points towards the edges of the design region for first-order models. All items in the list satisfied the necessary constraints. The standard exchange algorithm (see for instance Atkinson et al., 2007, ch. 12) was adapted so that we could incorporate the constraint that only twelve different oils could be used. Eight oils were used twice (rows 1-16 of $\mathbf{W}$) and four were used once. The algorithm operated as follows.

1. Pick 12 items at random from the candidate list of weights and assign the first to rows 1 and 2 of $\mathbf{W}$, the second to rows 3 and 4,..., the eighth to rows 15 and 16 and the final four to rows 17-20.

2. Randomly assign the elements of the columns of $\mathbf{P}$ (corresponding to the two process variables) to be -1 or 1.

3. Swap the first element in the candidate list for the first two rows of $\mathbf{W}$. Then evaluate the objective function (5.1) for each of the 16 possible combinations of the two process variables for runs 1 and 2. If the best of these is greater than the objective function value before the swap then retain the swap and the best settings of the process variables. If not then revert the swap. Repeat for all items in the candidate list.

4. Repeat the above down to rows 15 and 16 (the last of the repeated oils).

5. For rows 17-20 each oil is used only once so there are only four combinations of the process variables for which to evaluate the objective function.

6. Return to step 3 unless the objective function has not increased for an entire iteration.

The above algorithm was run 5000 times and resulted in several designs with the same highest objective function value. The final design was chosen from these on the basis of having good variance inflation factors (i.e., a lower level of multicollinearity amongst the factors). This is a sensible distinguishing criterion to use, since there are inherent correlations in the characteristic matrix **C** and hence there will be some degree of multicollinearity present in the design.

The final matrix [**W**|**P**] is given in Table 5.4. Notice how each pair of rows 1 and 2, 3 and 4, ..., 15 and 16 are identical for columns 1-11, since the first eight oils must be used twice. They do, however, have different combinations of load and roughness. Similarly, we notice how at most one ZDP is non-zero for each run and that there is only one non-zero dispersant for each run in keeping with the constraints. We also note that there is at most one detergent for each run. Although it was possible to mix detergents, preliminary investigations showed that the better designs did not use more than one detergent and hence items in the candidate list included at most one detergent.

The resulting scaled design (i.e., [**WC**|**P**] scaled to the range [-1,1]) is shown in Table 5.5. We notice the imbalance in some of the columns (e.g., ZN_APHOS) due to the constraints present (e.g., only one ZDP per run permitted). The column for roughness is also slightly unbalanced, with eleven rough discs being used. Notice that due to constraints, it is not possible to achieve the maximum desired level for ZN_PPHOS and hence there is no run for which the value in this column is 1.

The run order for the design in Table 5.5 was randomised and the experiment was carried out as described in Section 5.2.1.

Table 5.4: Percentages of each ingredient and settings of the two process variables in the 20-run design

Run	ZDP1	ZDP2	ZDP3	Antiwear	Disp1	Disp2	Det1	Det2	Det3	EP1	FM1	Load (N)	Roughness
1	0.42	0	0	0	2	0	0	3	0	0	0.1	37	Rough
2	0.42	0	0	0	2	0	0	3	0	0	0.1	72	Smooth
3	0	0.1	0	0	0	0	0	0	0	0	0.1	37	Smooth
4	0	0.1	0	0	0	0	0	0	0	0	0.1	72	Rough
5	0.42	0	0	0	0	4	0	0	0	0.1	0	37	Smooth
6	0.42	0	0	0	0	4	0	0	0	0.1	0	72	Rough
7	0	0	0.48	0.29	2	0	0	0	0	0.1	0.1	37	Rough
8	0	0	0.48	0.29	2	0	0	0	0	0.1	0.1	72	Smooth
9	0	0	0	0.47	0	4	0	0	3	0	0.1	37	Smooth
10	0	0	0	0.47	0	4	0	0	3	0	0.1	72	Rough
11	0	0.4	0	0	0	4	3	0	0	0.1	0.1	37	Rough
12	0	0.4	0	0	0	4	3	0	0	0.1	0.1	72	Smooth
13	0	0	0.48	0	0	4	0	3	0	0	0	37	Smooth
14	0	0	0.48	0	0	4	0	3	0	0	0	72	Rough
15	0	0	0.48	0.29	0	0	3	0	0	0	0	37	Rough
16	0	0	0.48	0.29	0	0	3	0	0	0	0	72	Smooth
17	0	0	0	0.47	0	0	0	3	0	0.1	0	37	Rough
18	0	0	0.48	0	0	0	0	0	3	0.1	0.1	37	Rough
19	0	0.4	0	0	2	0	0	0	3	0	0	37	Rough
20	0	0	0	0.12	2	0	3	0	0	0.1	0	72	Smooth

Table 5.5: Design matrix for 20-run experiment. All variables are scaled to lie in the region [-1,1]. Rough discs are coded 1 and smooth discs -1.

Run	ZN_APHOS	ZN_PPHOS	ZN_SPHOS	Phosphate Phos	Disp N	Disp B	Det CA	Det MG	Det TBN	EP	FM	Load	Roughness
1	-1	0.96	-1	-1	0.98	1	0.55	-1	0.5	-1	1	-1	1
2	-1	0.96	-1	-1	0.98	1	0.55	-1	0.5	-1	1	1	-1
3	-1	-1	-0.5	-1	-1	-1	-1	-1	-1	-1	1	-1	-1
4	-1	-1	-0.5	-1	-1	-1	-1	-1	-1	-1	1	1	1
5	-1	0.96	-1	-1	1	-1	-1	-1	-1	1	-1	-1	-1
6	-1	0.96	-1	-1	1	-1	-1	-1	-1	1	-1	1	1
7	1	-1	-1	0.21	0.98	1	-1	-1	-1	1	1	-1	1
8	1	-1	-1	0.21	0.98	1	-1	-1	-1	1	1	1	-1
9	-1	-1	-1	0.96	1	-1	-0.99	1	1	-1	1	-1	-1
10	-1	-1	-1	0.96	1	-1	-0.99	1	1	-1	1	1	1
11	-1	-1	1	-1	1	-1	1	-0.99	1	1	1	-1	1
12	-1	-1	1	-1	1	-1	1	-0.99	1	1	1	1	-1
13	1	-1	-1	-1	1	-1	0.55	-1	0.5	-1	-1	-1	-1
14	1	-1	-1	-1	1	-1	0.55	-1	0.5	-1	-1	1	1
15	1	-1	-1	0.21	-1	-1	1	-0.99	1	-1	-1	-1	1
16	1	-1	-1	0.21	-1	-1	1	-0.99	1	-1	-1	1	-1
17	-1	-1	-1	0.96	-1	-1	0.55	-1	0.5	1	-1	-1	1
18	1	-1	-1	-1	-1	-1	-0.99	1	1	1	1	-1	1
19	-1	-1	1	-1	0.98	1	-0.99	1	1	-1	-1	-1	1
20	-1	-1	-1	-0.51	0.98	1	1	-0.99	1	1	-1	1	-1

5.3 Two-stage analysis of data

For each run, a measurement of coefficient of friction was taken for 21 speeds. Up to measurement error, these speeds were the same for each run. These can then be plotted and interpolated to obtain 20 observed Stribeck curves. Four examples of the curves obtained are given in Figure 5.2. We take a two-stage modelling approach (see Davidian and Giltinan, 1995) whereby we

(i) model each curve separately

(ii) relate the model for each curve to the values of the factors.

Stage (i) is done using principal components and stage (ii) models the loadings for the principal components in terms of the factors varied in the experiment. This modelling approach requires two variance components; within and between run.

5.3.1 Using principal components analysis to model each observed Stribeck curve

The idea of the first stage of the modelling procedure is to obtain a model for each curve in a common form. This was achieved using principal components analysis (PCA).

Let $\mathbf{G}$ be a 21×20 matrix containing the observed Stribeck curve data points. We used singular value decomposition to express $\mathbf{G}$ as

$$\mathbf{G} = \mathbf{U}\mathbf{Z}\mathbf{V}^T, \tag{5.2}$$

where $\frac{1}{\sqrt{20}}\mathbf{U}\mathbf{Z}$ gives the principal components and $\sqrt{20}\mathbf{V}$ contains the loadings on each principal component for each run. The principal components are ordered so that they sequentially explain the highest proportion of variation in the observed Stribeck curves. Jolliffe (2002) gives further information on PCA.

In this case, the first four components explain 98.6% of the overall variation. The fifth component explains only an additional 0.5% and is also not in any way as interpretable as the first four components (see Section 5.3.3). Hence we model the

Stribeck curves using linear combinations of the first four principal components. The weights to use in the linear combinations are the loadings from (5.2).

Let $\mathbf{D}_j$ be the jth principal component (dimension 21×1) and l_{ij} be the loading for the ith run on the jth principal component. Then the model for the observed data for the ith run, $\mathbf{Y}_i$, can be written as

$$\mathbf{Y}_i = \sum_{j=1}^{4} \mathbf{D}_j l_{ij} + \mathbf{E}_i \,,$$

where $\mathbf{E}_i$ is a 21×1 vector of independent errors from $N(0, \sigma^2)$.

The first-stage fits for the four curves previously shown in Figure 5.2 are shown by the dashed line in Figure 5.3. Notice how all the fits are extremely close to the observed Stribeck curve, indicating a good fit for the first-stage models. It is highly desirable to have very good first-stage fits, since the models can only become less accurate at the second stage. The fits are equally good for both the convex and concave curves, and it appears that the principal components framework provides a set of models that are flexible enough to capture the variation in the response curves.

Due to the shape of the curves, there is evidence of very slight systematic under or over-estimation in some of the curves, but this is so small that it will not affect any conclusions drawn. The QQ-plot shown in Figure 5.4 indicates a slight departure from normality of the residuals. Again, since the residuals are so small (especially relative to the second stage residuals) this should not affect our conclusions.

5.3.2 How do the factors influence the Stribeck curves?

In the second stage of the modelling procedure, we model the loadings for the principal components in terms of the factors varied in the experiment. We fit the following models for $i = 1, \ldots, 20$ and $j = 1, \ldots, 4$.

$$l_{ij} = \mathbf{x}_i \boldsymbol{\beta} + f_{ij} \,, \tag{5.3}$$

where $\mathbf{x}_i$ denotes the ith run of a model matrix for the model we are fitting, $\boldsymbol{\beta}$ is a

Figure 5.3: Four example Stribeck curves (solid line) and their first-stage fits (dashed line)

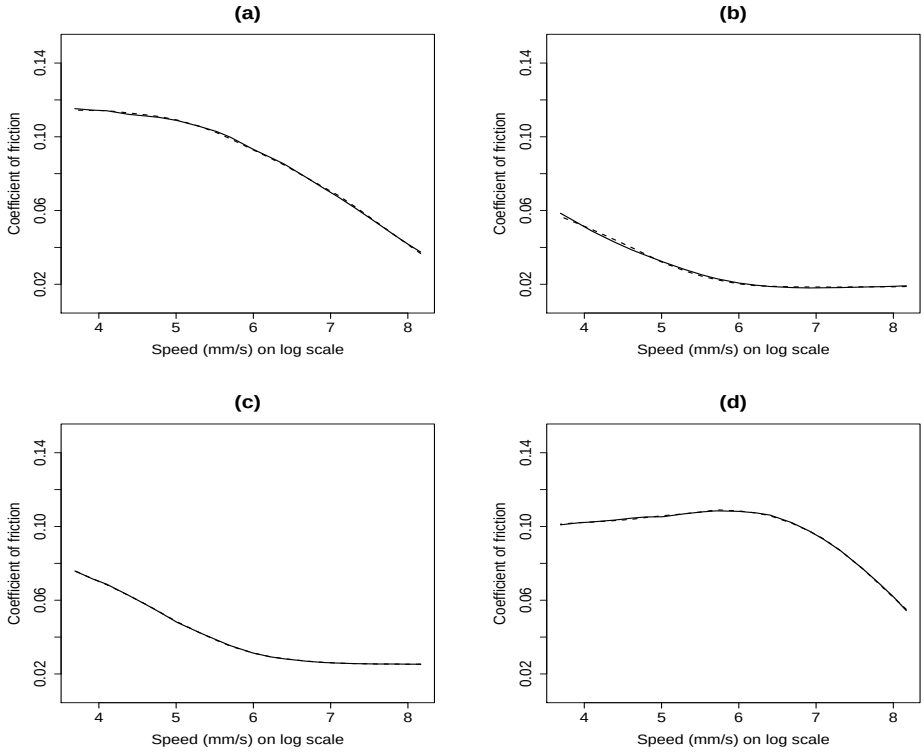
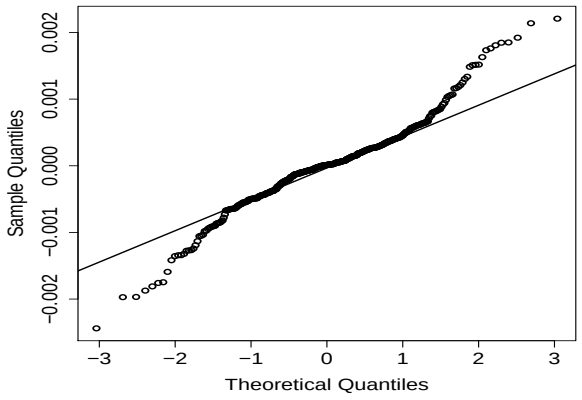


Figure 5.4: QQ-plot of first-stage residuals for all 20 runs



vector of unknown coefficients to be estimated from the data and f_{ij} is the second stage error on the loading for the jth principal component for the ith run. The vector of errors for the ith run, $(f_{i1}, f_{i2}, f_{i3}, f_{i4})$, is distributed as $MVN(0, \Delta)$. Note that this distribution does not depend on i.

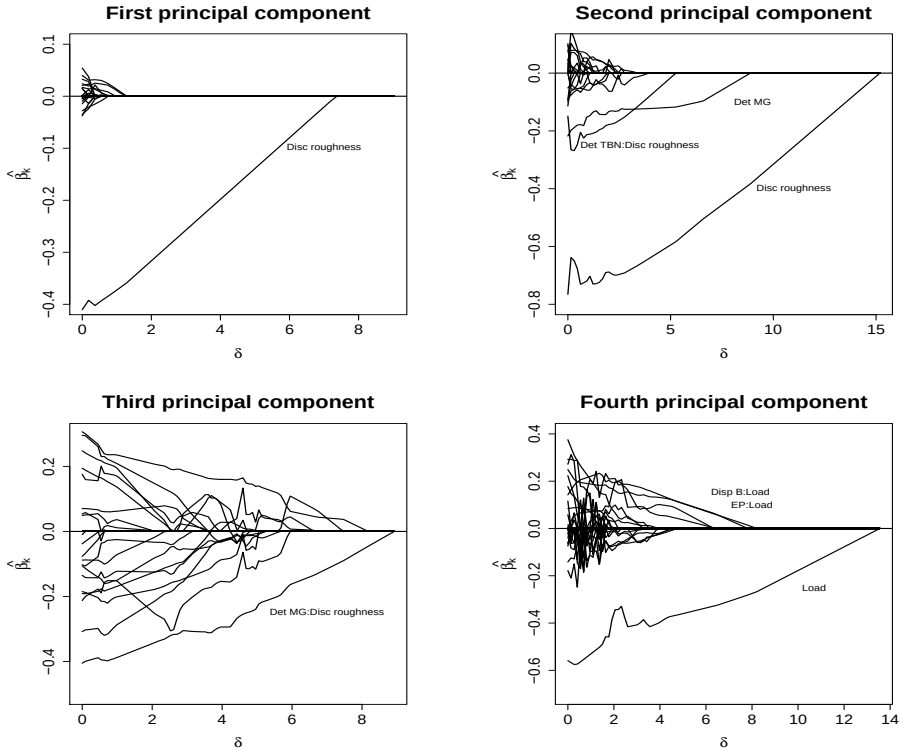
All the second stage models were fitted simultaneously using maximum likelihood estimation. The EM algorithm (Davidian and Giltinan, 1995, pp. 140) was used. This method allows correlations between the l_{ij} and within run variation to be incorporated. The separate least-squares fits were used as starting values of the algorithm.

Initially, the model matrix used in the fitting procedure incorporated an intercept and all main effects. However, from these second stage fits it was apparent that some interactions were present, particularly involving the process variable roughness. We needed to select a suitable model from the set of all main effects and two factor interactions (91 parameters in total). Because we have more parameters than runs, the data set is supersaturated. We therefore turned to a suitable method for analysing the output of supersaturated experiments. Several methods have been proposed in the literature, for instance, Westfall et al. (1998) suggested using forward selection, whilst Beattie et al. (2002) proposed a Bayesian model selection strategy. Further, Georgiou (2008) gave a method based on orthogonal decomposition. In this chapter, we use the Dantzig selector method, first proposed by Candes and Tao (2007) and then further explored by Phoa et al. (2009) in the form of the Gauss-Dantzig selector. Detailed comparisons of certain analysis methods by Marley and Woods (2010) showed the Gauss-Dantzig selector to be a highly effective method for detecting active effects in supersaturated problems. The Gauss-Dantzig selector is a more automated procedure than the original Dantzig selector; here we select important factors through examination of profile plots (see Yuan et al., 2007, for LARs).

The Dantzig selector belongs to a class of continuous variable selection techniques known as shrinkage methods, where each coefficient is shrunk towards zero at a different rate. The estimator $\hat{\boldsymbol{\beta}}$ is the solution to

$$\min_{\hat{\boldsymbol{\beta}} \in \mathbb{R}^k} ||\hat{\boldsymbol{\beta}}||_1 \quad \text{subject to} \quad ||\mathbf{X}^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})||_\infty \leq \delta\,. \tag{5.4}$$

Figure 5.5: Profile plots for each of the four principal components, plotting $\hat{\beta}_k$ against δ for each of the $k = 1, \ldots, 91$ parameters.



Here $||\boldsymbol{\beta}||_1 = |\beta_0| + \ldots + |\beta_m|$ is the l_1 norm, $||\boldsymbol{\beta}||_\infty = \max(|\beta_0|, \ldots, |\beta_m|)$ is the l_∞ norm, and δ is a tuning constant. The response vector is denoted by $\mathbf{y}$.

To implement the Dantzig selector, we reformulate (5.4) as a linear program and solve using the package `lpSolve` (Berkelaar, 2007) in `R` (R Development Core Team, 2009). We make a profile plot of $\hat{\beta}_k$ against δ for each of the $k = 1, \ldots, 91$ parameters and identify important effects by inspection of the profile plots, as proposed in Phoa et al. (2009). Such techniques are regularly used in shrinkage methods, such as LARS and LASSO.

We construct one profile plot for each of the four principal components. Performing model selection on each component individually will enable us to interpret specifically how each factor affects the shape of the Stribeck curve. The four profile plots are shown in Figure 5.5.

The profile plots show coefficient estimates for 100 evenly spaced values of δ. Effects which are still non-zero for high δ are generally thought to be active, particularly if they decay slowly towards zero. There are automated methods that can be used for

choosing an optimal δ, such as the AIC statistic or cross validation. Here, we use visual inspection since we wish to ensure we do not leave out any effects that may be marginally active. Leaving out an active factor at the screening stage is often less desired than carrying forward a spurious model term to the follow-up experiment, since the discarded factor will not be considered again.

For the first principal component there is one line on the plot which clearly corresponds to a significant effect, this being disc roughness. For the second component, disc roughness also appears to be highly significant (reaching zero at $\delta \approx 15$), whilst Det MG and the interaction between Det TBN and disc roughness may also be significant (reaching zero at $\delta \approx 9$ and $\delta \approx 5$). The third component is less clear, with no effect being clearly active. However, we retain the variable with consistently the largest coefficient - the interaction between Det MG and disc roughness. Such an interaction would be interpretable, since both main effects involved appeared to be active for the second component. For the fourth component, load was clearly an active factor, with the interaction between Disp B and load and also between EP and load being potentially active (both reaching zero at $\delta \approx 8$).

The terms identified as significant from the profile plots along with the main effects necessary for effect heredity to be obeyed were used to fit the second stage model. However, upon examining the fits, it was apparent that the level of bias in some of the fits was quite strong, see for instance Figure 5.6. Since the first loading on the first principal component controlled the height of the fitted curve (see Section 5.3.3), we examined further variables that could be marginally significant for the first principal component. Including the interaction between ZN_APHOS and disc roughness in the model for loadings on the first component reduced the level of bias in some of the fits and also reduced the overall mean squared error across all of the runs. Four fits including this interaction and the main effect of ZN_APHOS are shown in Figure 5.7. The dotted lines show the approximate 95% Wald confidence intervals, as described by Woods (2003, ch. 4). The estimate of the asymptotic covariance matrix for $\hat{\boldsymbol{\beta}}$ is given by Davidian and Giltinan (1995, ch. 5).

Notice how the bias in the fits for curves (a) and (d) has been reduced. All four of the example fits match the shape of the observed Stribeck curve very well. The

Figure 5.6: Two Stribeck curves (solid line) and their second-stage fits (dashed line) before the inclusion of the interaction of ZN_APHOS with disc roughness in the model. The fits display consistent bias.

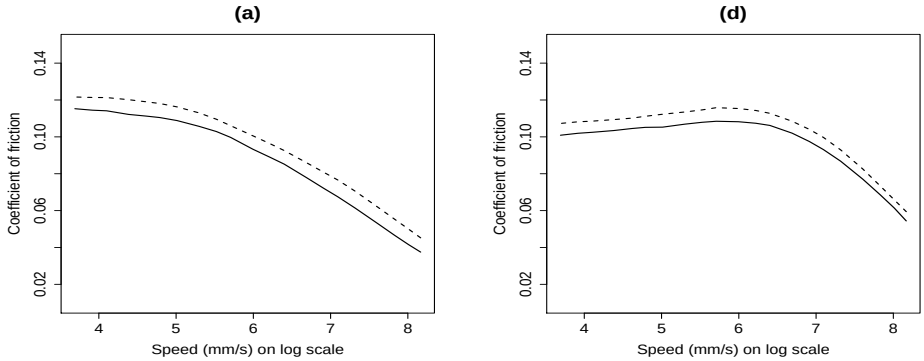


Figure 5.7: Four example Stribeck curves (solid line) and their second-stage fits (dashed line) with approximate 95% confidence intervals (dotted lines).

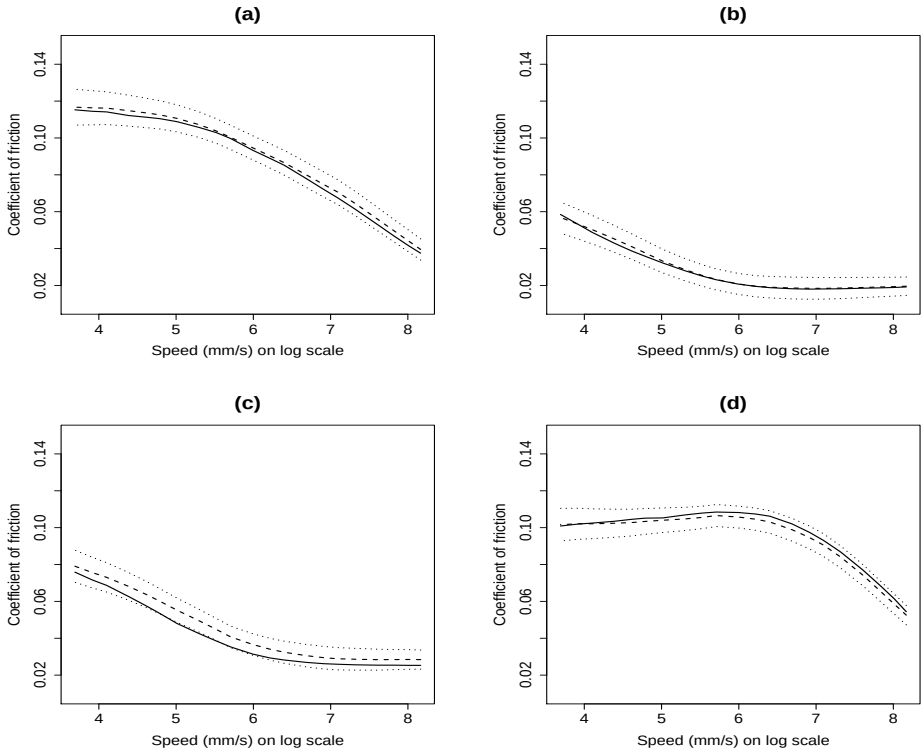
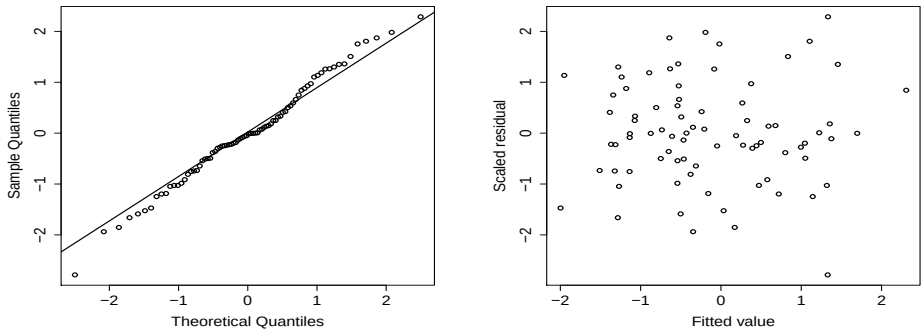


Figure 5.8: QQ-plot of scaled second-stage residuals and plot of scaled second-stage residuals against fitted values



confidence intervals were judged by subject experts to be narrow enough for the model to be useful. In the vast majority of the 20 runs, the fitted model captures very accurately the shape of the curve. Discrepancies between the fitted curve and the observed curve tend to come in the form of an upward or downward shift. This is due to the nature of the two-stage fitting procedure. For instance, a small error in the prediction of the loading for the first principal component will result in an upward or downward bias (see also Section 5.3.3).

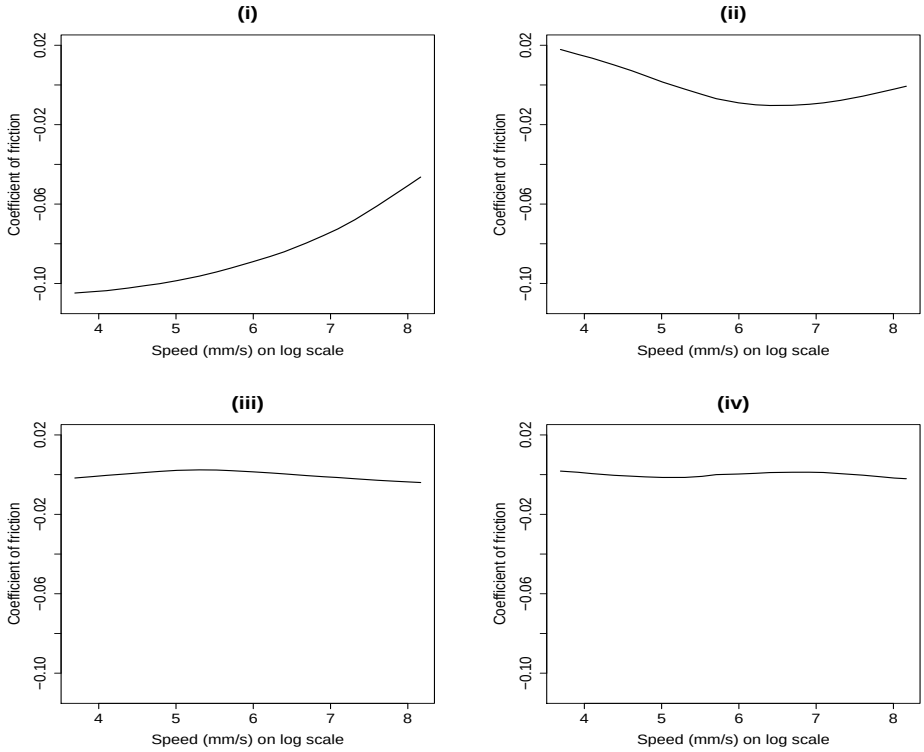
We now examine the residuals for the models fitted for the loadings at the second stage. Because of potentially unequal variance for the loadings for each component at the first stage, the residuals were transformed as in Grove et al. (2004) so that each quadruplet $(l_{ij} - \mathbf{x}_i\beta), j = 1, \ldots, 4$ had an approximately multivariate normal distribution with mean 0 and an identity covariance matrix. Figure 5.8 shows the QQ-plot of the scaled residuals and also a plot of the scaled residuals against fitted values; neither plot indicates serious departures from the model assumptions.

5.3.3 Interpretation of the principal components

Figure 5.9 shows plots of the first four principal components. Notice that components (i) and (ii) display much more curvature, as they are explaining a higher proportion of the variation in the shape of the Stribeck curves.

In this section, we describe how to interpret the principal components. For instance, if a particular factor is significant for a given principal component, we wish to know how this factor influences the shape of the observed Stribeck curve. We use a similar

Figure 5.9: Plots of the first four principal components.

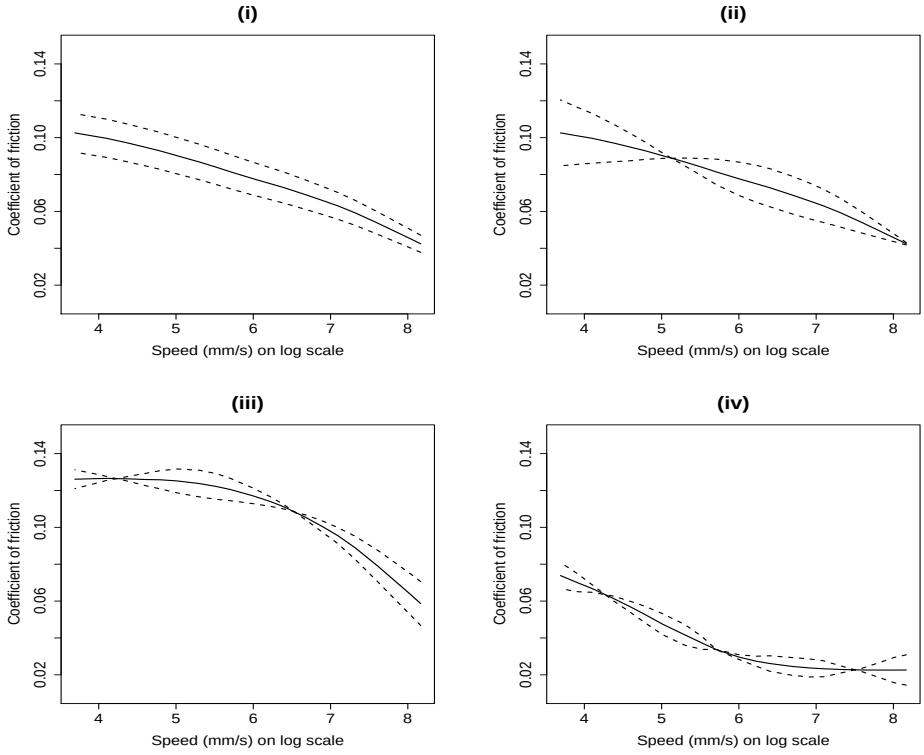


approach to one described in Campbell et al. (2006); each component is considered individually, see Figure 5.10. The solid line in Figure 5.10 (i) shows the mean of all 20 observed Stribeck curves. The upper (lower) dashed line is this mean minus (plus) a small multiple of the first component. This illustrates that the first component represents the general height of the Stribeck curve, and that variables significant for this component will change the overall height of the curve. For instance, rough discs tend to give higher curves than smooth discs.

The solid line in Figure 5.10 (ii) also shows the mean of all 20 observed Stribeck curves. The convex (concave) dashed line is this mean plus (minus) a small multiple of the second component. The loading on the second component is essentially determining whether or not we have a concave or convex curve (for example a curve like in Figure 5.2 (a) or (b)). The variable disc roughness is highly significant for the second component. Using a rough disc leads to a concave curve and using a smooth disc leads to a convex curve.

The third principal component is more interpretable when examining the concave curves (those obtained when using rough discs), hence the solid line in Figure 5.10

Figure 5.10: Plots illustrating the effect of a positive or negative loading on each of the first four principal components. For plots (i) and (ii) the solid line is the mean of all 20 observed Stribeck curves and the dashed lines are this mean ± a small multiple of the first and second components respectively. For plot (iii) the solid line is the mean of all observed Stribeck curves on the rough discs, and for plot (iv), the mean of all observed Stribeck curves on the smooth discs. Again, the dashed lines are these means ± a small multiple of the third and fourth components respectively

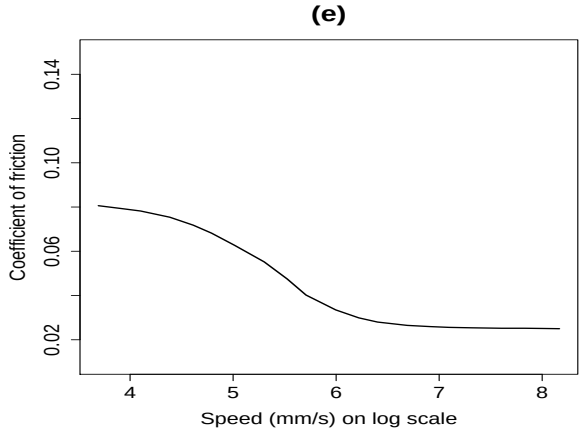


(iii) is the average of all the concave curves. Again, the dashed lines show this average ± a small multiple of the third component. The loading on this component seems to help establish the degree of curvature of the concave curves.

The fourth principal component tends to tidy up the fits, but its sizable loadings are more interpretable when examining the convex curves (those obtained when using smooth discs). The solid line in Figure 5.10 (iv) is this time the average of all the convex curves. The dashed lines show this average ± a small multiple of the fourth component. The fourth component seems to describe a small number of curves with a point of inflection (hence the component crossing zero on three occasions). This type of curve is shown in Figure 5.11.

More details on the effects of individual parameters are given in Section 5.5.

Figure 5.11: An observed Stribeck curve with a point of inflection.



5.4 Choosing follow-up runs

After the screening stage of the experiment, resource was available for 10 follow-up runs to help improve the model. In this section, we first describe the theory behind generating these follow-up runs, and then detail the actual runs used in the Stribeck curve example.

5.4.1 Theory

We first express the models we have fitted in matrix form. At the first-stage we fitted the model

$$\mathbf{Y}_i = \sum_{j=1}^{4} \mathbf{D}_j l_{ij} + \mathbf{E}_i \,.$$

In matrix form, this can be written as

$$\mathbf{Y} = [\mathbf{Y}_1^T, \ldots, \mathbf{Y}_{20}^T]^T = (\mathbf{I}_{20} \otimes \mathbf{D})\mathbf{L} + \mathbf{E}\,, \tag{5.5}$$

where, $\mathbf{I}_{20}$ is the 20×20 identity matrix, $\mathbf{D}$ is the 21×4 matrix with the four principal components as the columns. We have $\mathbf{E} = [\mathbf{E}_1^T, \ldots, \mathbf{E}_{20}^T]^T$ and set $\mathbf{L} = [\mathbf{L}_1, \ldots, \mathbf{L}_{20}]^T$, where $\mathbf{L}_i$ is the 1×4 vector of loadings for the ith run.

We let $\boldsymbol{\beta} = [\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_4]^T$, where $\boldsymbol{\beta}_j$ is a $1 \times p$ vector containing the coefficients for the loadings for the jth principal component and p is the total number of effects

under investigation. We use the notation $\mathbf{X}_i = \mathbf{I}_4 \otimes \mathbf{x}_i$, where $\mathbf{x}_i$ is the $1 \times p$ model matrix for the ith run, and let

$$\mathbf{X}^* = \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{20} \end{bmatrix}.$$

At the second stage, we then fit the model

$$\mathbf{L} = \mathbf{X}^* \boldsymbol{\beta} + \mathbf{F}\,, \tag{5.6}$$

where $\mathbf{F}$ is a 80×1 vector of errors.

Combining (5.5) and (5.6) we get

$$\mathbf{Y} = (\mathbf{I}_{20} \otimes \mathbf{D})\mathbf{X}^* \boldsymbol{\beta} + (\mathbf{I}_{20} \otimes \mathbf{D})\mathbf{F} + \mathbf{E}\,,$$

where $\mathbf{F} \sim MVN(0, \Sigma_F)$, with $\Sigma_F = \mathbf{I}_{20} \otimes \Delta$, and $\mathbf{E} \sim MVN(0, \Sigma)$, with $\Sigma = \sigma \mathbf{I}_{420}$. From the theory of generalised least squares, the information matrix is given by

$$\mathbf{X}^{*T}(\mathbf{I}_{20} \otimes \mathbf{D}^T)[(\mathbf{I}_{20} \otimes \mathbf{D})\Sigma_F(\mathbf{I}_{20} \otimes \mathbf{D}^T) + \Sigma]^{-1}(\mathbf{I}_{20} \otimes \mathbf{D})\mathbf{X}^*\,.$$

When designing the follow-up experiment, we wish to choose runs such that the determinant of the information matrix given the initial batch of runs is maximised. Let $\mathbf{X}_e^*$ be the model matrix for all the runs in the experiment (screening and follow-up) consisting of all the parameters found to be active, or at least, potentially active at the screening stage. The first 20 runs of $\mathbf{X}_e^*$ are fixed and we wish to choose the remaining 10 to maximise

$$\phi_D^{(2)} = |\mathbf{X}_e^{*T}(\mathbf{I}_{30} \otimes \mathbf{D}^T)[(\mathbf{I}_{30} \otimes \mathbf{D})\Sigma_F(\mathbf{I}_{30} \otimes \mathbf{D}^T) + \Sigma]^{-1}(\mathbf{I}_{30} \otimes \mathbf{D})\mathbf{X}_e^*|\,. \tag{5.7}$$

We use the best estimate of the basis (i.e., that from the screening stage) for generating the follow-up design. We extend the covariance matrices to be $\Sigma_F = \mathbf{I}_{30} \otimes \Delta$ and $\Sigma = \sigma \mathbf{I}_{630}$ and estimate Δ and σ from the data from the screening stage. Such an approach makes best use of information from screening stage when generating the follow-up runs.

Table 5.6: Percentages of each ingredient and settings of the two process variables in the 10-run follow-up design

Run	ZDP3	Det1	Det2	Det3	Disp1	EP1	Load (N)	Roughness
1	0.48	0	0	3	2	0	72	Smooth
2	0.48	0	0	3	2	0.1	72	Rough
3	0	0	0	0	2	0	72	Rough
4	0.48	0	0	0	2	0	37	Smooth
5	0	0	0	3	2	0.1	37	Smooth
6	0.48	3	0	0	2	0.1	37	Smooth
7	0.48	0	0	0	0	0	37	Rough
8	0.48	3	0	0	2	0.1	72	Rough
9	0.48	0	0	3	0	0.1	72	Smooth
10	0	0	0	0	0	0	72	Smooth

5.4.2 Experimental design for 10 follow-up runs

For the follow-up runs, there were no constraints on the total number of oils that could be used. A total of 7 factors out of the initial 13 were retained, along with 5 interactions, see Section 5.3.2. The 10 follow-up runs were generated using a similar algorithm to the one described in Section 5.2 to maximise the objective function (5.7). The matrix giving the weights for the ingredients and the settings of the process variables for the follow-up runs is given in Table 5.6.

The amount of the ingredients that did not influence levels of any of the factors retained for the follow-up runs was zero for all runs, except for the amount of antiwear. This was set so that the minimum required level of phosphorous was always achieved, in line with constraint 3. Notice that the columns for the two process variables are now balanced, when the 30 runs are considered as a whole. We also note that Detergent 2 is never included in the oil. This is because we can achieve a higher level of the factor Det TBN combined with a low/high level of Det MG by using Detergent 1 or 3.

The resulting scaled design is shown in Table 5.7. The follow-up design places the factor ZN_APHOS at its high level more times than in the screening experiment, which overall makes the column more balanced. It is possible to do this now that we are only considering one ZDP in the follow-up design (since ZDP1 and ZDP2 do not affect the levels of any of the factors retained for the follow-up experiment). We

Table 5.7: Design matrix for 10-run follow-up experiment. All variables are scaled to lie in the region [-1,1]. Rough discs are coded 1 and smooth discs -1.

Run	ZN_APHOS	Det MG	Det TBN	Disp B	EP	Load	Roughness
1	1	1	1	1	-1	1	-1
2	1	1	1	1	1	1	1
3	-1	-1	-1	1	-1	1	1
4	1	-1	-1	1	-1	-1	-1
5	-1	1	1	1	1	-1	-1
6	1	-0.99	1	1	1	-1	-1
7	1	-1	-1	-1	-1	-1	1
8	1	-0.99	1	1	1	1	1
9	1	1	1	-1	1	1	-1
10	-1	-1	-1	-1	-1	1	-1

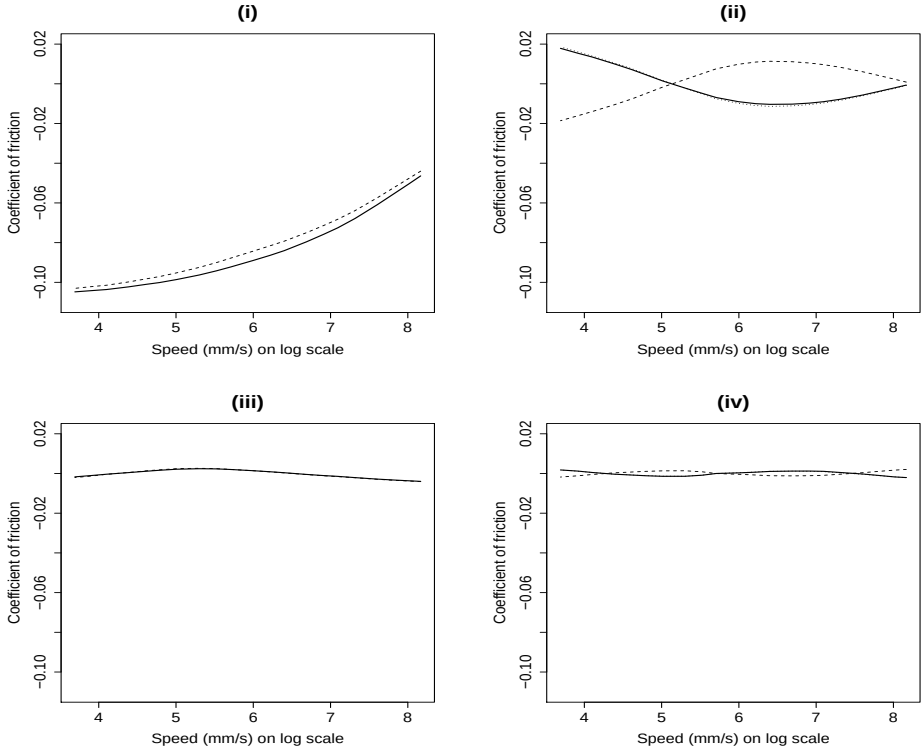
see a similar trend with the level of Disp B.

5.5 Results of follow-up runs

The 10 runs shown in Table 5.7 were randomised and the experiment carried out. The predictions based on the model obtained from the initial 20 runs were compared to the curves observed in the 10 follow-up runs. They were found to fit well, except for run 5, which produced an unexpectedly high curve. A repeat was run and the observed Stribeck curve was closer to the prediction in terms of shape, but still decidedly biased. The larger than expected bias could be due to the MTM receiving its annual calibration between the follow-up runs and the repeat. Due to this bias, run 5 was excluded from the analysis.

The principal components were recalculated for the remaining 29 runs and plotted as the dashed line in Figure 5.12. The solid line shows the principal components based on the first 20 runs. For components i and iii (where the dashed line is masked by the solid line) we see very little change between 20 and 29 runs. For components ii and iv, the component from 29 runs is virtually exactly the 20 run component multiplied by minus one (shown by the dotted line overlapping the solid line). Thus the components are virtually identical, with the interpretation of the direction of the effects reversed for components ii and iv. We use the components from the full

Figure 5.12: Plots of the first four principal components based on 20 (solid) and 29 (dashed) runs. For components ii and iv, the dotted line shows the component based on 29 runs multiplied by minus one.

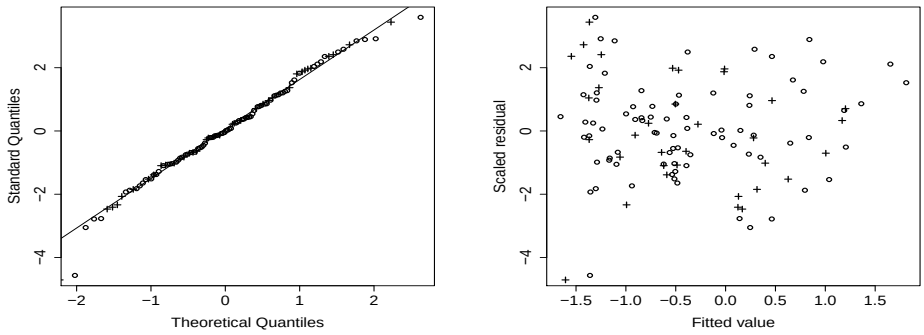


29 runs for the remainder of the analysis.

Second stage models were estimated for all 29 curves, using all the effects carried forward to the follow-up experiment. All 12 of these effects could be argued as being at least potentially active for some principal components, based on examining box-plots of the loadings. Therefore, it was difficult to reduce the number of parameters in the model. The most obviously active effects were disc roughness, load and the interactions between Det MG and disc roughness and Det TBN and disc roughness. Fitting a model in these effects and also the main effects of Det MG and Det TBN (to obey effect heredity) resulted in an increase in mean squared error of 248%, strongly indicating that the remaining effects were appreciably improving the fit.

The residual plots shown in Figure 5.13 show no discernible patterns or deviations from normality. The points indicated by a cross symbol denote those relating to the follow-up runs. There is no detectable difference between the follow-up runs and the screening runs.

Figure 5.13: QQ-plot of scaled second-stage residuals and plot of scaled second-stage residuals against fitted values based on 29 runs. Circular points correspond to runs 1-20 and crosses correspond to the nine retained follow-up runs.



We now examine graphically the effects of changing some of the factor levels. Figure 5.14 (left) shows the estimated effect on the Stribeck curve of changing the level of Det MG from -0.99 (dashed line) to 1 (solid line) when a smooth disc is being used and all other factors are kept constant. Figure 5.14 (right) shows the corresponding effect when a rough disc is being used. The difference between the curves is much greater when a rough disc is used, due to the substantive interaction between Det MG and disc roughness.

We also examine the effect of changing load from low to high. Load was active only for the fourth principal component, which explained only a small amount of the variation in the shape of the Stribeck curves. Therefore, Figure 5.15 shows only small differences between the estimated curves for low and high load.

Disp B was included in the model due to it's interaction with load. The plots in the upper row of Figure 5.16 show that, at a high load, Disp B is likely to have little effect on the shape of the Stribeck curve. However, at low loads (plots in the bottom row of Figure 5.16) the difference is more noticeable, with a lower level of Disp B appearing to produce lower curves at low speeds.

5.6 Discussion

We have described the statistical methodology behind an investigation into the effect of certain factors on the shape of Stribeck curves. The models that were estimated during this work and the graphical displays of anticipated effects of changing various

Figure 5.14: The effect of changing the level of Det MG from -0.99 to 1 on smooth and rough discs.

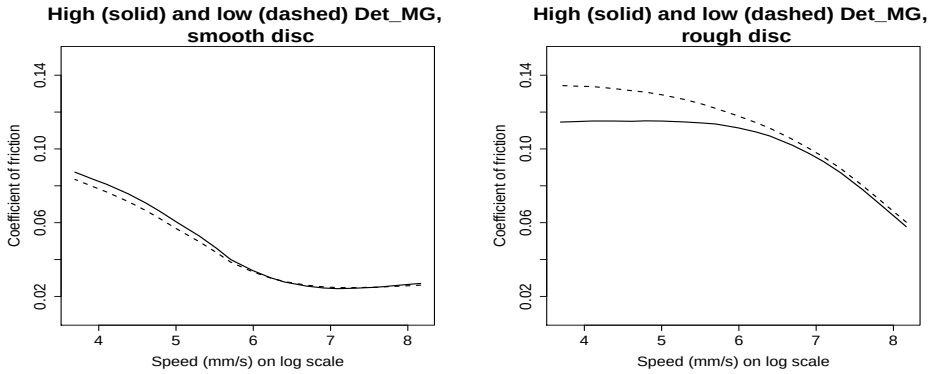


Figure 5.15: The effect of changing the level of load from -1 to 1 on smooth and rough discs.

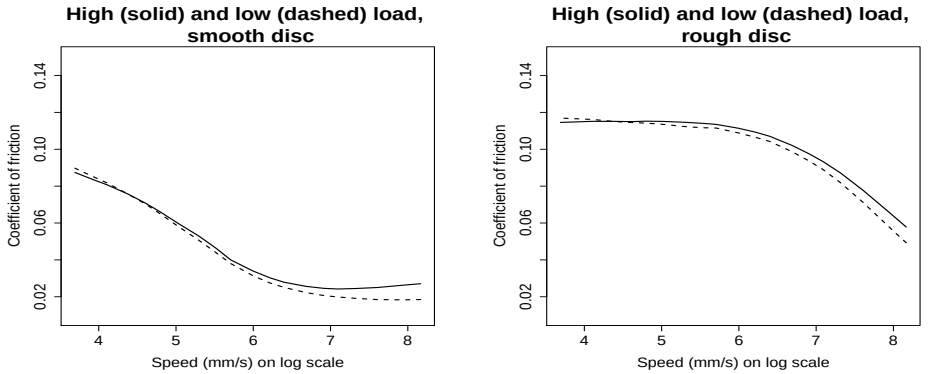
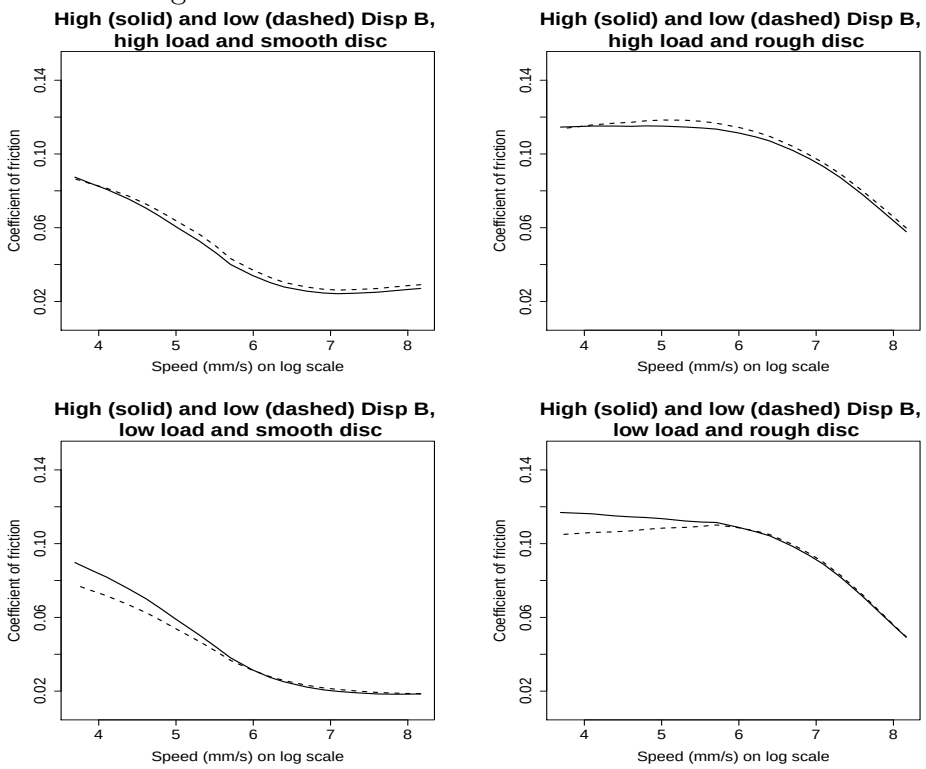


Figure 5.16: The effect of changing the level of Disp B from -1 to 1 on smooth and rough discs with high or low load.



factors were found to be useful to the chemists involved in the project. We conclude this work with a brief discussion of repeatability of results, validation of the models and areas requiring further investigation.

Two runs from the screening stage of the experiment(runs 1 and 2) were run again to establish the repeatability of the observed Stribeck curves. Both runs involved the same oil but different settings of the two process variables. The two observed curves from the screening experiment are indicated by the solid lines in Figure 5.17. Their repeats are plotted as the dashed lines. We see a small error in the repeat runs (particularly in plot (a)). This error is only slightly smaller than the level of bias we see in some of the fitted curves, hence confirming the usefulness of the fitted model.

The company also performed two further runs, using factor settings that were not used in any of the previous runs. The observed curves for these runs (solid line) and their predicted curves (dashed line) are displayed in Figure 5.18. The predicted curves can be seen to match the observed curves very well. There is a small amount of

Figure 5.17: Observed Stribeck curves for runs 1 and 2 (a and b) from the screening stage (solid lines) and their repeats (dashed lines)

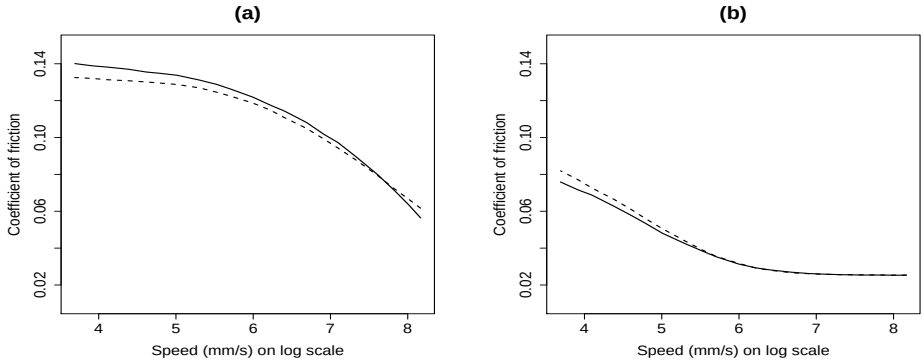
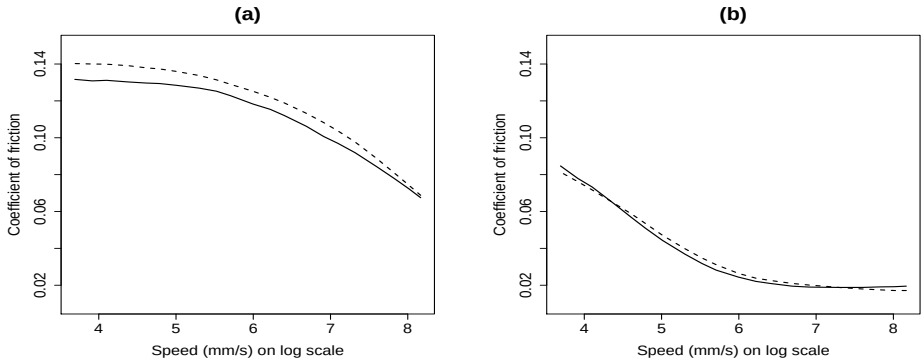


Figure 5.18: Observed Stribeck curves from two validation runs (solid lines) and their predicted curves (dashed lines)



bias evident in curve (a) but this is not too much larger than the errors seen between repeat runs in Figure 5.17. We note, however, that there are limited conclusions that can be drawn from only two validation runs and that more validation runs would give us more confidence in the fitted model.

Discussion with researchers at Lubrizol revealed that the small amounts of bias seen in the fitted curves could be due to some discs being slightly more rough or smooth than others, even within their respective groups. Roughness of the discs can be quantified by calculating different summary measures from a roughness profile, a plot of depth measurements obtained by running a stylus across a portion of the disc. Two useful measurements which were identified were R_a, the average absolute deviation from the mean line of the measurements in the profile, and R_{sk}, the skewness of the profile measurements. Roughness profiles were taken in three positions on all discs prior to experimentation but were found to vary considerably

within the same disc. Consequently, it was not possible to accurately characterise disc roughness using R_a and R_{sk}. Models were fitted using R_a instead of a two-level disc roughness factor, but these were found to provide a less accurate fit to the data, along with wider confidence intervals. Obtaining better ways to measure disc roughness is the subject of further investigation.

It should be noted that, ideally, the experimenters would have anticipated a small number of strong two-factor interactions, and the screening experiment could then have been designed with the model matrix, $\mathbf{X}$ also incorporating two-factor interactions. This would then be a supersaturated design problem, with there being more parameters to be investigated than runs available in the experiment. Bayesian D-optimality (Jones et al., 2008) could potentially have been used as a suitable criterion.

We also point out that if, at the screening stage of the experiment, we had more runs available than observations per Stribeck curve, then the whole experiment could, under some assumptions, be designed in the framework described in Section 5.4. Suppose there are q points which make up each Stribeck curve and that $q < n$. Let's assume that we will select all principal components to form our basis, so that $\mathbf{E} = \mathbf{0}$ (i.e. no first stage errors). Also assume that the loadings are uncorrelated. Then $\Sigma_F = \mathbf{I}_{n\times q}$. The objective function to find the 20 screening runs becomes

$$|\mathbf{X}^T(\mathbf{I}_{20} \otimes \mathbf{D}^T)[(\mathbf{I}_{20} \otimes \mathbf{D})(\mathbf{I}_{20} \otimes \mathbf{D}^T)]^{-1}(\mathbf{I}_{20} \otimes \mathbf{D})\mathbf{X}|\,.$$

Since we are using all available principal components, $\mathbf{D}$ is a $q \times q$ square matrix and hence the objective function reduces to

$$|\mathbf{X}^T\mathbf{X}|\,.$$

Even though in the example considered in this chapter we have $q > n$, maximising $|\mathbf{X}^T\mathbf{X}|$ is still a sensible option, particularly since we do not know the principal components in advance.

Lubrizol were particularly encouraged by the findings of this experiment, and there are now plans for them to apply this methodology to other similar projects.

Chapter 6

Overall conclusions and future work

This thesis has discussed industrial screening experiments and has provided new methods and insights for the design and analysis of supersaturated experiments. The performance of the supersaturated designs has been evaluated by calculating the power and type I error rate across a variety of simulation studies. New applications of supersaturated experiments have been presented. These include supersaturated experiments where factor levels cannot be set independently, and robust product design via supersaturated experiments. Finally a real-life screening experiment run by The Lubrizol Corporation to investigate the influence of factors on friction, represented by Stribeck curves was discussed. This example involved the development of a new method of selecting follow-up designs for two-stage models.

6.1 Conclusions

Results of a detailed simulation study have enabled recommendations to be made for the successful application of supersaturated designs. The recommendation of most potential use to practitioners is that the number of factors should not normally exceed twice the number of runs. The study also showed that, despite often being unbalanced, Bayesian D-optimal designs can perform well, and tend to have slightly higher power in return for a slightly higher type I error rate when compared to $E(s^2)$-optimal designs.

A suitable method for analysing the results of supersaturated experiments has also

been identified. Compared to two other existing methods the Gauss-Dantzig selector had consistently higher power and also a low type I error rate across a range of scenarios and experiment sizes. The Gauss-Dantzig selector also performed better than a newly proposed model-averaging procedure.

Advances have also been made in the design of supersaturated experiments. A compound criterion has been proposed for designing supersaturated experiments that facilitates the construction of designs with both low levels of multicollinearity and good accuracy of parameter estimators. The criterion maximises an objective function that combines the average variance inflation factor with a modification of the A-optimality objective function. This criterion is different to the majority of existing criteria in that it considers projections into more than two factors. It also has the advantage that all models containing up to a pre-specified number of factors can be estimated. In principal it can be used for constructing designs for any number of runs and factors. This new criterion can be especially effective for experiments where the levels of the factors cannot be set independently of one another. Reducing multicollinearity is useful in such experiments, since there may be inherent relationships between the factors in the candidate list of design points. Therefore we recommend using this criterion for such experiments.

It has been demonstrated that to which columns of a supersaturated design the active factors are assigned can have a considerable impact on the ability to detect those factors in the analysis. Investigation revealed that for a given design, active factors assigned to columns with high average variance inflation factors were far more likely to be declared inactive in the analysis compared to those assigned to columns with low variance inflation factors. It was therefore suggested that experimenters may wish to consider this issue, and assign factors to columns carefully, using any available prior information. A method for doing this was proposed, which involved assigning the factors using the average variance inflation factor for individual columns of the design.

One especially useful application of screening in industry is in the context of robust product design experiments and it has been shown that supersaturated designs can be very effective for this problem. Using a criterion which is focussed only on the

aliasing structure for effects of interest proved more effective than using existing criteria for constructing such designs. Large improvements in the power to detect active factors can be gained, especially when there are more noise factors than control factors. Often, potential noise factors (and hence potential control by noise interactions) are ignored in such experiments, because noise factors can be expensive to vary in experiments. The implementation of supersaturated designs can enable more noise factors to be investigated and hence improve products further. The criterion proposed in Chapter 4 is also generalisable outside of the robust parameter design setting to applications where there is a set of effects which is of interest and a set which is not.

The work in this thesis was strongly motivated by interactions with industry and Chapter 5 described a real screening experiment to investigate the impact of factors on functional responses, namely Stribeck curves. Designing the experiment using a candidate list approach and analysing via a two-stage model, with principal components analysis used at the first stage, proved to be effective. Several active factors were identified, and accurate models for the Stribeck curves were obtained. A novel method for constructing a follow-up experiment was described and implemented.

6.2 Future work

There are a variety of open issues and areas of future work resulting from this thesis. In Chapter 2 we could include a Bayesian analysis method in the comparisons, such as the two-stage model selection strategy proposed by Beattie et al. (2002). The comparisons could also be extended to scenarios where we also aim to detect active two-factor interactions.

In order to speed up generation of the designs using the compound criterion described in Chapter 3, and to enable the generation of larger designs, it would be beneficial to develop updating formulae for the objective function when an exchange or coordinate exchange algorithm is being used. This would ideally avoid the inversion of the large number of matrices currently required, which could result in computational savings. As an example, Atkinson et al. (2007, ch. 12) present a repeated application of the Sherman-Morrison formula (Sherman and Morrison, 1950)

for when D-optimality is being used as the criterion. It is, however, unclear what savings in computer time would be possible for the objective function in Chapter 3, since the matrices to be inverted are typically small. As a further extension, the criterion in Chapter 3 could also be applied to models with interactions.

For the example in Chapter 5, it may be possible to create a candidate-list-free continuous optimisation approach to generate the optimal elements of the weight matrix $\mathbf{W}$. This will most likely be more computationally intensive, but would have the advantage of being a more general method.

Additional work could involve investigating screening experiments for more complicated models. This thesis has described screening experiments for only main effects and, in some cases, two-factor interactions. For some experiments, modelling the response may require more complex functions of the controllable factors, for example quadratic effects or spline bases, for which new methodology may be required.

References

Abraham, B., Chipman, H., and Vijayan, K. (1999), "Some risks in the construction and analysis of supersaturated designs," *Technometrics*, 41, 135–141.

Allen, T. T. and Bernshteyn, M. (2003), "Supersaturated designs that maximise the probability of identifying active factors," *Technometrics*, 45, 90–97.

Aston, J. A. D., Chiou, J.-M., and Evans, J. P. (2010), "Linguistic pitch analysis using functional principal component mixed effect models," *Journal of the Royal Statistical Society Series C*, 59, 297–317.

Atkinson, A. C., Donev, A. N., and Tobias, R. D. (2007), *Optimum experimental designs, with SAS*, Oxford: Oxford University Press.

Ballistreri, F. P., Fortuna, C. G., Musumarra, G., Pavone, D., and Scire, S. (2002), "Principal properties (PPs) as solvent descriptors for multivariate optimization in organic synthesis: specific PPs for ethers," *Arkivoc*, 11, 54–64.

Beattie, S. D., Fong, D. K. H., and Lin, D. K. J. (2002), "A two-stage Bayesian model selection strategy for supersaturated designs," *Technometrics*, 44, 55–63.

Berkelaar, M. (2007), *lpSolve: Interface to Lp_solve v. 5.5 to solve linear/integer programs.*

Booth, K. H. V. and Cox, D. R. (1962), "Some systematic supersaturated designs," *Technometrics*, 4, 489–495.

Box, G. E. P. (1959), "Discussion of the papers of Satterthwaite and Budne," *Technometrics*, 1, 174–180.

Box, G. E. P. and Meyer, R. D. (1986), "An analysis for unreplicated fractional factorials," *Technometrics*, 28, 11–18.

Burnham, K. P. and Anderson, D. R. (2002), *Model selection and multimodel inference*, New York, London: Springer, 2nd ed.

Campbell, K., McKay, M. D., and Williams, B. J. (2006), "Sensitivity analysis when model outputs are functions," *Reliability Engineering and System Safety*, 91, 1468–1472.

Candes, E. and Tao, T. (2007), "The Dantzig selector: statistical estimation when p is much larger than n," *The Annals of Statistics*, 35, 2313–2351.

Chen, J. and Liu, M. Q. (2008), "Optimal mixed-level supersaturated design with general number of runs," *Statistics and Probability Letters*, 78, 2496–2502.

Cook, R. D. and Nachtsheim, C. J. (1980), "A comparison of algorithms for constructing exact D-optimal designs," *Technometrics*, 22, 315–324.

Crosier, R. B. (2000), "Some new two-level saturated designs," *Journal of Quality Technology*, 32, 103–110.

Davidian, M. and Giltinan, D. M. (1995), *Nonlinear models for repeated measurement data*, London: Chapman and Hall.

Dean, A. M. and Lewis, S. M. (2006), *Screening: methods for experimentation in industry, drug discovery, and genetics*, New York: Springer.

Deng, L. Y., Lin, D. K. J., and Wang, J. (1996), "A measurement of multi-factor orthogonality," *Statistics & Probability Letters*, 28, 203–209.

Dowson, D. (1998), *History of tribology, 2nd ed.*, London and Bury St Edmunds: Professional Engineering Publishing.

DuMouchel, W. and Jones, B. (1994), "A simple Bayesian modification of D-optimal designs to reduce dependence on an assumed model," *Technometrics*, 36, 37–47.

Georgiou, S. D. (2008), "Modelling by supersaturated designs," *Computational Statistics and Data Analysis*, 53, 428–435.

Gilmour, S. G. (2006), "Supersaturated designs in factor screening," in *Screening: methods for experimentation in industry, drug discovery, and genetics*, eds. Dean, A. M. and Lewis, S. M., New York: Springer, pp. 169–190.

Grove, D. M., Woods, D. C., and Lewis, S. M. (2004), "Multifactor B-spline mixed models in designed experiments for the engine mapping problem," *Journal of Quality Technology*, 36, 380–391.

Holcomb, D. R., Montgomery, D. C., and Carlyle, W. M. (2007), "The use of supersaturated experiments in turbine engine development," *Quality Engineering*, 19, 17–27.

Jolliffe, I. T. (2002), *Principal component analysis*, New York: Springer, 2nd ed.

Jones, B., Lin, D. K. J., and Nachtsheim, C. J. (2008), "Bayesian D-optimal supersaturated designs," *Journal of Statistical Planning and Inference*, 138, 86–92.

Jones, B. and Nachtsheim, C. J. (2009), "D-Efficient designs with minimal aliasing," Tech. rep., University of Minnesota.

Jones, B. A., Li, W., Nachtsheim, C. J., and Ye, K. Q. (2009), "Model-robust supersaturated and partially supersaturated designs," *Journal of Statistical Planning and Inference*, 139, 45–53.

Kang, L. and Joseph, V. R. (2009), "Bayesian optimal single arrays for robust parameter design," *Technometrics*, 51, 250–261.

Läuter, E. (1974), "Experimental design in a class of models," *Mathematische Operationsforschung und Statistik*, 5, 379–398.

Lewis, S. M. and Dean, A. M. (2001), "Detection of interactions in experiments on large numbers of factors," *Journal of the Royal Statistical Society Series B*, 63, 633–672.

Li, P., Zhao, S., and Zhang, R. (2010), "A cluster analysis selection strategy for supersaturated designs," *Computational Statistics and Data Analysis*, 54, 1605–1612.

Li, R. and Lin, D. K. J. (2002), "Data analysis in supersaturated designs," *Statistics & Probability Letters*, 59, 135–144.

— (2003), "Analysis methods for supersaturated design: some comparisons," *Journal of Data Science*, 1, 249–260.

Li, W. W. and Wu, C. F. J. (1997), "Columnwise-pairwise algorithms with applications to the construction of supersaturated designs," *Technometrics*, 39, 171–179.

Lin, D. K. J. (1993), "A new class of supersaturated designs," *Technometrics*, 35, 28–31.

— (1995), "Generating systematic supersaturated designs," *Technometrics*, 37, 213–225.

— (1998), "Spotlight interaction effects in main-effect plans: a supersaturated design approach," *Quality Engineering*, 11, 133–139.

Liu, M. Q. and Lin, D. K. J. (2009), "Construction of optimal mixed-level supersaturated designs," *Statistica Sinica*, 19, 197–211.

Liu, Y., Ruan, S., and Dean, A. M. (2007), "Construction and analysis of Es^2 efficient supersaturated designs," *Journal of Statistical Planning and Inference*, 137, 1516–1529.

Loeppky, J. L., Bingham, D., and Sitter, R. (2006), "Constructing non-regular robust parameter designs," *Journal of Statistical Planning and Inference*, 136, 3710–3729.

Lu, X., Khonsari, M. M., and Gelinck, E. R. M. (2006), "The Stribeck curve: experimental results and theoretical prediction," *Journal of Tribology*, 128, 789–794.

Madigan, D. and Raftery, A. E. (1994), "Model selection and accounting for model uncetainty in graphical models using Occam's window," *Journal of the American Statistical Association*, 89, 1535–1546.

Marley, C. J. and Woods, D. C. (2010), "A comparison of design and model selection methods for supersaturated experiments," *Computational Statistics and Data Analysis*, 54, 3158–3167.

Meyer, R. D., Steinberg, D. M., and Box, G. (1996), "Follow-up designs to resolve confounding in multifactor experiments," *Technometrics*, 38, 303–313.

Meyer, R. K. and Nachtsheim, C. J. (1995), "The coordinate-exchange algorithm for constructing exact optimal experimental designs," *Technometrics*, 37, 60–69.

Miller, A. (2002), *Subset selection in regression*, Boca Raton: Chapman and Hall.

Miller, A., Sitter, R. R., Wu, C. F. J., and Long, D. (1993), "Are large Taguchi-style experiments necessary? A reanalysis of gear and pinion data," *Quality Engineering*, 6, 21–37.

Morris, M. D. (2006), "An overview of group factor screening," in *Screening: methods for experimentation in industry, drug discovery, and genetics*, eds. Dean, A. M. and Lewis, S. M., New York: Springer, pp. 191–206.

Neter, J., Kutner, M. H., Nachtsheim, C. J., and Wasserman, W. (1996), *Applied statistical linear models*, Chicago: The McGraw-Hill Companies, Inc., 4th ed.

Nguyen, N. K. (1996), "An algorithmic approach to constructing supersaturated designs," *Technometrics*, 38, 69–73.

Nguyen, N. K. and Cheng, C. S. (2008), "New $E(s^2)$-optimal supersaturated designs constructed from incomplete block designs," *Technometrics*, 50, 26–31.

O'Hagan, A. and Forster, J. J. (2004), *Kendall's advanced theory of statistics Vol. 2B: Bayesian Inference*, London: Arnold, 2nd ed.

Phoa, F. K. H., Pan, Y. H., and Xu, H. (2009), "Analysis of supersaturated designs via the Dantzig selector," *Journal of Statistical Planning and Inference*, 139, 2362–2372.

Plackett, R. L. and Burman, J. P. (1946), "The design of optimum multifactorial experiments," *Biometrika*, 33, 305–325.

Put, R., Xu, Q. S., Massart, D. L., and Vander Heyden, Y. (2004), "Multivariate adaptive regression splines (MARS) in chromatographic quantitative structure-retention relationship studies," *Journal of Chromatography A*, 1055, 11–19.

R Development Core Team (2009), *R: A language and environment for statistical computing*, R Foundation for Statistical Computing, Vienna, Austria.

Ramsay, J. O. and Silverman, B. W. (2005), *Functional data analysis*, New York: Springer, 2nd ed.

Russell, K. G., Lewis, S. M., and Dean, A. M. (2004), "Fractional factorial designs for the detection of interactions between design and noise factors," *Journal of Applied Statistics*, 31, 545–552.

Ryan, K. J. and Bulutoglu, D. A. (2007), "$E(s^2)$-optimal supersaturated designs with good minimax properties," *Journal of Statistical Planning and Inference*, 137, 2250–2262.

Satterthwaite, F. (1959), "Random balance experimentation," *Technometrics*, 1, 111–137.

Sherman, J. and Morrison, W. J. (1950), "Adjustment of an inverse matrix corresponding to a change in one element of a given matrix," *Annals of Mathematical Statistics*, 21, 124–127.

Shoemaker, A. C., Tsui, K. L., and Wu, C. F. J. (1991), "Economical experimentation methods for robust design," *Technometrics*, 33, 415–427.

Snee, R. D. (1973), "Techniques for the analysis of mixture data," *Technometrics*, 15, 517–528.

Sojoudi, H. and Khonsari, M. M. (2010), "On the behavior of friction in lubricated point contact with provision for surface roughness," *Journal of Tribology*, 132, 012102.

Srivastava, J. N. (1975), "Designs for searching non-negligible effects," in *A survey of statistical design and linear models*, ed. Srivastava, J. N., Amsterdam: North-Holland Publishing Co., pp. 507–519.

Stribeck, R. (1902), "Kugellager für beliebige belastungen," *Zeitschrift des Vereines Deutscher Ingenieure*, 46, 1341–1348; 1432–1438; 1463–1470.

Taguchi, G. (1986), *Introduction to quality engineering: designing quality into products and processes*, Tokyo: Asian Productivity Organization.

Vine, A. E., Lewis, S. M., Dean, A. M., and Brunson, D. (2008), "A critical assessment of two-stage group screening through industrial experimentation," *Technometrics*, 50, 15–25.

Watson, G. S. (1961), "A study of the group screening method," *Technometrics*, 3, 371–388.

Welch, W. J., Yu, T. K., Kang, S. M., and Sacks, J. (1990), "Computer experiments for quality control by parameter design," *Journal of Quality Technology*, 22, 15–22.

Westfall, P. H., Young, S. S., and Lin, D. K. J. (1998), "Forward selection error control in the analysis of supersaturated designs," *Statistica Sinica*, 8, 101–117.

Woods, D. C. (2003), "Designing experiments for polynomial spline models," Ph.D. thesis, University of Southampton.

Wu, C. F. J. (1993), "Construction of supersaturated designs through partially aliased interactions," *Biometrika*, 80, 661–669.

Wu, C. F. J. and Hamada, M. (2000), *Experiments: Planning, Analysis, and Parameter Design Optimization*, New York: Wiley.

Wu, C. F. J. and Zhu, Y. (2003), "Optimal selection of single arrays for parameter design experiments," *Statistica Sinica*, 13, 1179–1199.

Xu, H. and Wu, C. F. J. (2005), "Construction of optimal multi-level supersaturated designs," *The Annals of Statistics*, 33, 2811–2836.

Yamada, S. and Lin, D. K. J. (1999), "Three-level supersaturated designs," *Statistics & Probability Letters*, 45, 31–39.

Yuan, M., Joseph, V. R., and Lin, Y. (2007), "An efficient variable selection approach for analyzing designed experiments," *Technometrics*, 49, 430–439.

Zhu, Y., Zeng, P., and Jennings, K. (2007), "Optimal compound orthogonal arrays and single arrays for robust parameter design experiments," *Technometrics*, 49, 440–453.